Existence and approximation for a 3D model of thermally-induced phase transformations in shape-memory alloys

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This note deals with a three-dimensional model for thermal stress-induced transformations in shape-memory materials. Microstructure, like twined martensites, is described mesoscopically by a vector of internal variables containing the volume fractions of each phase. The problem is formulated mathematically within the energetic framework of rate-independent processes. An existence result is proved and we study space-time discretizations and establish convergence of these approximations.

1 Mathematical formulation

We consider a material with a reference configuration $\Omega \subset \mathbb{R}^d$ with $d \in \{2, 3\}$. This body may undergo displacements $u : \Omega \to \mathbb{R}^d$ and phase transformations. The latter will be characterized by a mesoscopic internal variable $z : \Omega \to Z$ where Z is the Gibbs simplex, associated with the N pure phases $\widehat{e}_1, \ldots \widehat{e}_N \in \mathbb{R}^N$, where $\widehat{e}_j$ is the jth unit vector, i.e., $Z \overset{\text{def}}{=} \text{conv}\{\widehat{e}_1, \ldots, \widehat{e}_N\}$. The set of admissible displacements $\mathcal{F}$ is chosen as a suitable subspace of $\mathrm{H}^1(\Omega; \mathbb{R}^d)$ by prescribing Dirichlet data on the subset Γ_{Dir} of $\partial\Omega$. The physical displacement is $u + u_{\text{Dir}}$, where $u_{\text{Dir}} : [0, T] \to \mathrm{H}^1(\Omega; \mathbb{R}^d)$ is prescribed a priori. We consider here the extension of $u_{\text{Dir}}(t)$ to Ω, but actually only the trace on Γ_{Dir} would be needed. The internal variable z lives in $\mathcal{Z} \overset{\text{def}}{=} \big\{ z \in \mathrm{H}^1(\Omega; \mathbb{R}^N) \,|\, z(x) \in Z \text{ a.e. } x \in \Omega \big\}$. We assume also that the material behavior depends on the temperature θ, which will be considered as a time dependent given parameter. Therefore we will not solve an associated heat equation but we will treat θ as an applied load and we denote it by $\theta_{\text{appl}} : [0, T] \times \Omega \to [\theta_{\min}, \theta_{\max}]$. This approximation for the temperature is used in engineering models and is justified when the changes of the loading are slow and the body is small in at least one direction: in such a case, excess of heat can be transported very fast to the surface of the body and then radiated into the environment. The linearized strain tensor is given by $\mathbf{e}(u) \overset{\text{def}}{=} \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$. The *stored-energy potential* takes the following form

$$\mathcal{E}(t, u, z) \overset{\text{def}}{=} \int_\Omega \Big(W(\mathbf{e}(u + u_{\text{Dir}}(t)), z, \theta_{\text{appl}}(t)) + \frac{\sigma}{2} |\nabla z|^2 \Big) \, \mathrm{d}x - \langle l(t), u \rangle, \tag{1.1}$$

where the stored-energy density $W(\mathbf{e}(u + u_{\text{Dir}}(t)), z, \theta_{\text{appl}}(t))$ describes the material behavior. Here σ is a positive coefficient that is expected to measure some nonlocal interaction effect for the internal variable z and $l(t)$ denotes an applied mechanical loading. The total dissipation distance between two internal states $z_0, z_1 \in \mathcal{Z}$ is defined via

$$\mathcal{D}(z_0, z_1) \overset{\text{def}}{=} \int_\Omega D(z_0 - z_1) \, \mathrm{d}x, \tag{1.2}$$

where D is a quasi-distance, namely

$$D(z_0, z_1) = 0 \quad \Longleftrightarrow \quad z_0 = z_1 \quad \text{and} \quad \forall\, z_1, z_2, z_3 \in Z : \; D(z_1, z_3) \le D(z_1, z_2) + D(z_2, z_3). \tag{1.3}$$

Finally our problem is assumed to be governed by the *energetic formulation* of rate independent processes as introduced in $[1, 2, 4, 5]$. A function $(u, z) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ is called an *energetic solution* of the rate-independent problem associated with $\mathcal{E}$ and $\mathcal{D}$ if for all $t \in [0, T]$, the *global stability condition* (S) and the *global energy balance* (E) are satisfied, i.e.

(S) $\forall (\bar{u}, \bar{z}) \in \mathcal{F} \times \mathcal{Z} : \; \mathcal{E}(t, u(t), z(t)) \le \mathcal{E}(t, \bar{u}, \bar{z}) + \mathcal{D}(z(t), \bar{z})$,

(E) $\mathcal{E}(t, u(t), z(t)) + \text{Var}_{\mathcal{D}}(z; [0, t]) = \mathcal{E}(0, u(0), z(0)) + \int_0^t \partial_s \mathcal{E}(s, u(s), z(s)) \, \mathrm{d}s$,

where $\text{Var}_{\mathcal{D}}(z; [0, t]) \overset{\text{def}}{=} \sup\big\{ \sum_1^n \mathcal{D}(z(t_{j-1}), z(t_j)) \,\big|\, n \in \mathbb{N}, \; 0 \le t_0 < t_1 < \ldots < t_n \le t \big\}$ for all $t \in [0, T]$.

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2 Existence result and convergence of the space-time discretization

We assume that $\theta_{\rm appl} \in \mathrm{C}^1([0,T];\mathrm{L}^\infty(\Omega;[\theta_{\min},\theta_{\max}]))$, $l \in \mathrm{C}^1([0,T];(\mathrm{H}^1(\Omega;\mathbb{R}^d))')$ and $u_{\rm Dir} \in \mathrm{C}^1([0,T];\mathrm{H}^1(\Omega;\mathbb{R}^d))$. Moreover, we impose that $W(\cdot,z,\theta)$ is strictly convex, $W, \partial_\theta W$ and $\partial_e W$ are continuous functions and that there exist C, c, C_0^W, C_1^W, C^θ, C_0, C_1, C^e, $c_1, c_2 > 0$, $\widehat{p} \in (0,2)$, and a nondecreasing function $\omega : [0,\infty) \to [0,\infty)$ with $\lim_{\tau\to 0^+}\omega(\tau) = 0$ such that we have

$$
\begin{aligned}
&c\big(|e|^2{+}|z|^2\big) - C \le W(e,z,\theta) \le C\big(|e|^2{+}|z|^2\big) + C,\\
&|\partial_e W(e,z,\theta)|^2 + |\partial_\theta W(e,z,\theta)| \le C_1^W\big(W(e,z,\theta){+}C_0^W\big),\\
&\big|\partial_e W(e,z,\theta_1){-}\partial_e W(e,z,\theta_2)\big|^2 + \big|\partial_\theta W(e,z,\theta_1){-}\partial_\theta W(e,z,\theta_2)\big| \le C_1\big(W(e,z,\theta_1){+}C_0\big)\,\omega(|\theta_1{-}\theta_2|),\\
&\big|\partial_\theta W(e_1,z_1,\theta){-}\partial_\theta W(e_2,z_2,\theta)\big| \le C^\theta(|e_1{-}e_2|{+}|z_1{-}z_2|)(1{+}|e_1{+}e_2|{+}|z_1{+}z_2|),\\
&\big|\partial_e W(e_1,z_1,\theta){-}\partial_e W(e_2,z_2,\theta)\big| \le C^e(|e_1{-}e_2|{+}|z_1{-}z_2|),\\
&|W(e,z_1,\theta){-}W(e,z_2,\theta)| \le C(1{+}|e|)^{\widehat{p}}\omega(|z_1{-}z_2|),\\
&c_1|z_1{-}z_2| \le D(z_1,z_2) \le c_2|z_1{-}z_2|.
\end{aligned}
$$

We use the abstract result of [1] to prove the existence result given in the following Theorem.

Theorem 2.1 *Assume that W, D, $u_{\rm Dir}, l$, $\theta_{\rm appl}$ satisfy the assumptions from above and let $(u_0,z_0) \in \mathcal{F}\times\mathcal{Z}$ be stable for $t=0$. Then there exists an energetic solution $(u,z) : [0,T] \to \mathcal{F}\times\mathcal{Z}$ such that $(u_0,z_0) = (u(0),z(0))$ and $u \in \mathrm{L}^\infty([0,T];\mathrm{H}^1(\Omega;\mathbb{R}^d))$ and $z \in \mathrm{L}^\infty([0,T];\mathrm{H}^1(\Omega;Z)) \cap \mathrm{BV}([0,T];\mathrm{L}^1(\Omega;Z))$.*

Notice that we do not have uniqueness of solutions for the full problem. Hence we cannot expect convergence of the whole approximation sequence, but we can obtain convergence of subsequences to solutions of the full problem. For the time discretization we consider $\tau \in (0,T)$ and a partition $\Pi^\tau = \{0 = t_0^\tau < t_1^\tau < \ldots < t_{k^\tau}^\tau = T\}$ with $t_k^\tau - t_{k-1}^\tau \le \tau$ for $k = 1,\ldots,k^\tau$. For the spatial discretization we choose a set of length parameters $h>0$ accumulating at $h=0$ and let $\mathcal{F}_h$ and V_h be closed subspaces of $\mathcal{F}$ and $\mathrm{H}^1(\Omega;\mathbb{R}^N)$, respectively and let $\mathcal{Z}_h = \{z_h \in V_h \,|\, z_h(x) \in Z \text{ a.e. in } \Omega\}$. We assume that the sets $\mathcal{F}_h\times\mathcal{Z}_h$ satisfy the *standard density assumption*, namely for all $(u,z) \in \mathcal{F}\times\mathcal{Z}$, there exists (u_h,z_h) such that

$$
(u_h,z_h) \in \mathcal{F}_h\times\mathcal{Z}_h \quad\text{and}\quad (u_h,z_h)\to(u,z) \quad\text{strongly}\quad\text{in}\quad \mathcal{F}\times\mathcal{Z}. \tag{2.1}
$$

We approximate the initial condition (u_0,z_0) by $[(u_0,z_0)]^h \in \mathcal{F}_h\times\mathcal{Z}_h$ and we consider the following incremental problems:

$$
(\mathrm{IP})^{\tau,h} \quad \begin{cases} \text{for } k=1,\ldots,k^\tau \text{ find}\\ (u_k^{\tau,h}, z_k^{\tau,h}) \in \mathrm{Argmin}\big\{\mathcal{E}(t_k^\tau,\widehat{u}^h,\widehat{z}^h) + \mathcal{D}(z_{k-1}^{\tau,h},\widehat{z}^h)\,|\,(\widehat{u}^h,\widehat{z}^h)\in\mathcal{F}_h\times\mathcal{Z}_h\big\}. \end{cases}
$$

The approximate solution $(\bar{u}^{\tau,h},\bar{z}^{\tau,h}) : [0,T] \to \mathcal{F}\times\mathcal{Z}$ is defined as the right-continuous piecewise constant (cf. [3]) and has the desirable properties, namely, the sequence of approximants is precompact (which can be understood as the "stability of the numerical algorithm") and any limit point of the sequence of approximants is an energetic solution for the rate-independent system (which can be understood as "consistency of the numerical algorithm").

Theorem 2.2 ***(Convergence of the approximate solution).*** *Assume that* (2.1) *and the assumptions of Theorem 2.1 hold and let $[(u_0,z_0)]^h \in \mathcal{F}\times\mathcal{Z}$ be such that $[(u_0,z_0)]^h \to (u_0,z_0)$ in $\mathcal{F}\times\mathcal{Z}$. Then, there exists a subsequence $(\bar{u}^{\tau_n,h_n},\bar{z}^{\tau_n,h_n})$ which converges to a solution (u,z) of* (S) *and* (E) *with $(u(0),z(0)) = (u_0,z_0)$ such that for all $t\in[0,T]$, we have*

$$
\begin{aligned}
&(\bar{u}^{\tau_n,h_n}(t),\bar{z}^{\tau_n,h_n}(t)) \to (u(t),z(t)) \quad \textit{strongly} \quad \textit{in} \quad \mathcal{F}\times\mathcal{Z},\\
&\mathcal{E}(t,\bar{u}^{\tau_n,h_n}(t),\bar{z}^{\tau_n,h_n}(t)) \to \mathcal{E}(t,u(t),z(t)), \qquad \mathrm{Var}_{\mathcal{D}}(\bar{z}^{\tau_n,h_n};[0,t]) \to \mathrm{Var}_{\mathcal{D}}(z;[0,t]).
\end{aligned}
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