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

Adrien Petrov

Weierstraß-Institute für Angewandte Analysis und Stochastik

joint work with Alexander Mielke and Laetitia Paoli

DFG Research Center MATHEON
Mathematics for key technologies

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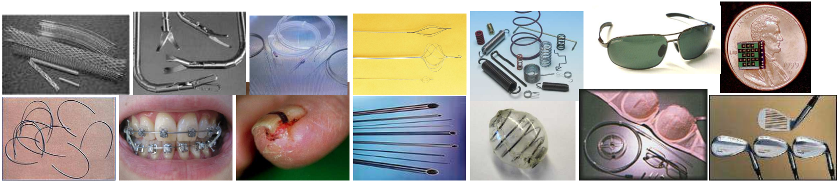
Weierstraß-Institut für Angewandte Analysis und Stochastik

Shape-memory alloys

Shape-memory alloys are used because of their

- shape memory under heating and cooling,
- superelastic properties under mechanical loading,
- hysteretic behavior for damping of vibrations.

Applications: medical, space applications, MEMS...



AIM: Model that describes the evolution of phase mixtures

Pure phases can be measured experimentally:

$z \in \{\underbrace{e_1}_{\text{mart1}}, \dots, \underbrace{e_k}_{\text{martk}}, \dots, \underbrace{e_N}_{\text{aust}}\} \subset \mathbb{R}^N$

energy functionals

$W(\mathbf{E}, e_j),\ j = 1, \dots, N$

Mixtures $z \in Z = \mathrm{conv}\{e_1, \dots, e_N\}$ is the Gibbs simplex
$W(\mathbf{E}, z) : \mathbb{R}^{d\times d}_{\mathrm{sym}} \times Z \to \mathbb{R}$ is the mixture function called the free-energy of mixing by Govindjee, Hackl & Heinen'07

State variables		**Applied fields**	
$u : \Omega \to \mathbb{R}^d$	displacement	$\ell_{\mathrm{appl}} : [0, T] \to \mathcal{F}^*$	mechanical loading
$z : \Omega \to Z$	phase mixture	$\theta_{\mathrm{appl}} : [0, T] \times \Omega \to \mathbb{R}$	temperature given

u_{Dir}: the time-dependent Dirichlet boundary data

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State variables

$u : \Omega \to \mathbb{R}^d$ displacement

$z : \Omega \to Z$ phase mixture

Applied fields

$\ell_{\mathrm{appl}} \in \mathrm{C}^1([0, T]; \mathrm{H}^1(\Omega; \mathbb{R}^d)')$

$\theta_{\mathrm{appl}} \in \mathrm{C}^1([0, T]; \mathrm{L}^\infty(\Omega; [\theta_{\min}, \theta_{\max}]))$

$u_{\mathrm{Dir}} \in \mathrm{C}^1([0, T]; \mathrm{H}^1(\Omega; \mathbb{R}^d))$

Energy: $\mathcal{E}(t,u,z) = \int_\Omega \big(W(x,e(u+u_{\mathrm{Dir}}(t)),z,\theta(t)) + \frac{\sigma}{2}|\nabla z|^2\big)\,\mathrm{d}x - \langle \ell(t),u\rangle$
where $e(u) = \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$ is the infinitesimal strain

Dissipation distance: $\mathcal{D}(z_1, z_2) = \int_\Omega \psi(x, z_2 - z_1)\,\mathrm{d}x$
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Mielke & Theil'04.
$(u,z) : [0,T] \to \mathcal{F} \times \mathcal{Z}$ is called **energetic solution**, if

(S) $\mathcal{E}(t,u(t),z(t)) \le \mathcal{E}(t,\widetilde{u},\widetilde{z}) + \mathcal{D}(z(t),\widetilde{z})$ for all $(\widetilde{u},\widetilde{z}) \in \mathcal{F} \times \mathcal{Z}$

(E) $\mathcal{E}(t,u(t),z(t)) + \mathrm{Var}_{\mathcal{D}}(z;[0,t]) = \mathcal{E}(0,u_0,z_0) + \int_0^t \partial_s \mathcal{E}(\cdot,u,z)\,\mathrm{d}s$

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Previous works:

- Govindjee, Mielke & Hall'03
- Souza, Mamiya & Zouain'98, Auricchio & Petrini'04, Mielke & P.'07

Assumptions on W**.** Let $\omega : [0,\infty) \to [0,\infty)$ be a nondecreasing function with $\lim_{\tau\to 0^+}\omega(\tau) = 0$ such that

$W(\cdot, z, \theta)$ is strictly convex,

$W, \partial_\theta W \in \mathrm{C}^0(\mathbb{R}^{d\times d}_{\mathsf{sym}} \times Z \times [\theta_{\min}, \theta_{\max}]; \mathbb{R})$

$\partial_e W \in \mathrm{C}^0(\mathbb{R}^{d\times d}_{\mathsf{sym}} \times Z \times [\theta_{\min}, \theta_{\max}]; \mathbb{R}^{d\times d}_{\mathsf{sym}})$

$c\big(|e|^2+|z|^2\big) - C \le W(e,z,\theta) \le c\big(|e|^2+|z|^2\big) + C$

$|\partial_e W(e,z,\theta)|^2 + |\partial_\theta W(e,z,\theta)| \le C_1^W\big(W(e,z,\theta)+C_0^W\big)$

$\big|\partial_\theta W(e,z,\theta_1)-\partial_\theta W(e,z,\theta_2)\big| \le C_1^\theta\big(W(e,z,\theta_1)+C_0^\theta\big)\,\omega(|\theta_1-\theta_2|)$

$\big|\partial_e W(e,z,\theta_1)-\partial_e W(e,z,\theta_2)\big|^2 \le C_1^e\big(W(e,z,\theta_1)+C_0^e\big)\,\omega(|\theta_1-\theta_2|)$

$\big|\partial_\theta W(e_1,z_1,\theta)-\partial_\theta W(e_2,z_2,\theta)\big| \le C^\theta(|e_1-e_2|+|z_1-z_2|)(1+|e_1+e_2|+|z_1+z_2|)$

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Assumption on $\mathcal{D}$**.** $c_1|z_1-z_2| \le D(z_1,z_2) \le c_2|z_1-z_2|$

Theorem (The Existence result)

Under the assumptions on W and ψ given above. Let $(u(0), z(0))$ satisfies ***(S)****. Then there exists $(u, z) : [0, T] \to \mathcal{F} \times \mathcal{Z}$ satisfying* ***(S)&(E)*** *such that*

$$u \in \mathrm{L}^{\infty}([0, T]; \mathrm{H}^1(\Omega; \mathbb{R}^d))$$
$$z \in \mathrm{L}^{\infty}([0, T]; \mathrm{H}^1(\Omega; Z))$$
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If W is α-uniformly convex jointly in the first two arguments then (u, z) is Lipschitz continuous

Finite-element spaces $\mathcal{F}_h \subset \mathcal{F}$ and $\mathcal{Z}_h \subset \mathcal{Z}$, time step $\tau > 0$
Density assumption: $\underbrace{(u_h, z_h)}_{\in \mathcal{F}_h \times \mathcal{Z}_h} \to (u, z)$ strongly in $\mathcal{F} \times \mathcal{Z}$

Space-Time Discretization

(IP) $^{h,\tau}$

$$q_k^{h,\tau} \in \underset{\widehat{q}^h \in \mathcal{F}_h \times \mathcal{Z}_h}{\mathrm{Argmin}} \left(\mathcal{E}(t_k^\tau, \widehat{q}^h) + \mathcal{D}(z_{k-1}^{h,\tau}, \widehat{z}^h) \right)$$

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Like Backward Euler for the heat equation:

$$u_t + \Delta u = 0 \qquad u_k^{h,\tau} \in \underset{\widehat{u}}{\mathrm{Argmin}} \Big(\int_\Omega \tfrac{1}{2} |\nabla \widehat{u}|^2 \,\mathrm{d}x + \frac{1}{2(t_k - t_{k-1})} \|\widehat{u} - u_{k-1}^{h,\tau}\|^2 \Big)$$

Piecewise constant interpolants $\overline{q}^{h,\tau}(t) = (\overline{u}^{h,\tau}, \overline{z}^{h,\tau}) : [0, T] \to \mathcal{F}_h \times \mathcal{Z}_h$

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AIM: investigate the asymptotics as $h \to 0$ and $\tau \to 0$

Convergence of the space-time discretization follows from

- ▷ uniform a priori estimates ⇝ *numerical stability*
- ▷ accumulation points are solutions ⇝ *consistency*

Previous works: Mielke'05, Roubíček & Mielke'06

Theorem (Convergence of the space-time discretization)

Under the assumptions given above. Then there exists a subsequence $\overline{q}^{h,\tau} = (\overline{u}^{h,\tau}, \overline{z}^{h,\tau})$ *which converges to a solution* (u, z) *of* ***(S)&(E)*** *and*

$$u \in \mathrm{L}^\infty([0,T];\mathrm{H}^1(\Omega;\mathbb{R}^d))$$
$$z \in \mathrm{L}^\infty([0,T];\ \mathrm{H}^1(\Omega;Z))$$
$$z \in \mathrm{BV}([0,T];\mathrm{L}^1(\Omega;Z))$$

such that

$$\overline{q}^{h_n,\tau_n}(t) \to q(t) \text{ strongly in } \mathcal{F} \times \mathcal{Z}$$
$$\mathcal{E}(t,\overline{q}^{h_n,\tau_n}(t)) \to \mathcal{E}(t,q(t))$$
$$\mathrm{Var}_{\mathcal{D}}(\overline{q}^{h_n,\tau_n};[0,t]) \to \mathrm{Var}_{\mathcal{D}}(q;[0,t])$$

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- include rate-dependent effects like a heat equation
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Thank you for your attention !

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