C18 Analysis and numerics of multidimensional models for elastic phase transformations in shape-memory alloys

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Mathematics for key technologies

W I A S
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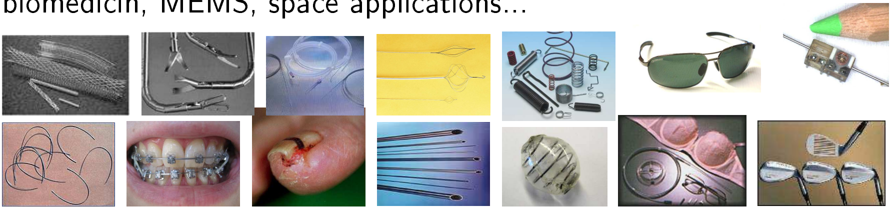
Background

Shape-memory alloys are used because of their

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

Applications:
biomedicin, MEMS, space applications...



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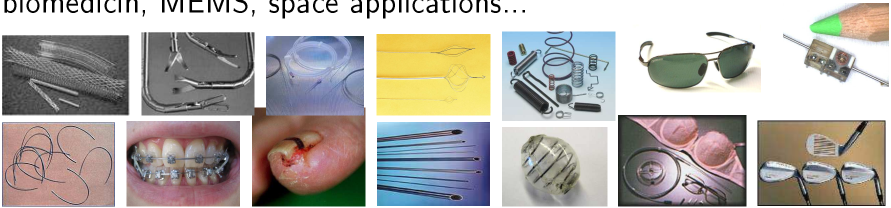
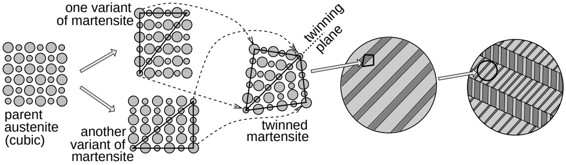


AIM: Find good mathematical models (analysis and numerics)

Background of SMAs

The functionality of SMAs have their origin in microstructures, which evolve under thermal or mechanical loading



NEED: Model that describes 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

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

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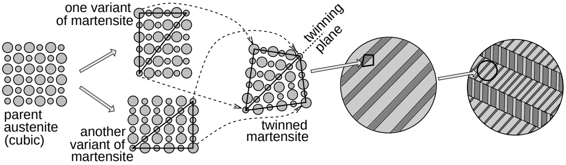

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mixtures $z \in Z := \mathrm{conv}\{e_1, \ldots, e_N\} \subset \mathbb{R}^N$ (Z = Gibbs' simplex)

$$W: \begin{cases} \mathbb{R}^{d\times d}_{\mathrm{sym}} \times Z \to \mathbb{R}, \\ (\mathbf{E}, z) \mapsto W(\mathbf{E}, z), \end{cases}$$

mixture function (see also **C13**)

State variables

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

$z : \Omega \to Z$ phase indicator

Applied fields

$\ell_{\rm appl} : [0, T] \to \mathcal{F}^*$ mechan. loading

$\theta_{\rm appl} : [0, T] \times \Omega \to \mathbb{R}$ temperature

Energy: $\mathcal{E}(t, u, z) = \int_\Omega W(\nabla u, z, \nabla z, \theta_{\rm appl}(t))\,\mathrm{d}x - \langle \ell_{\rm appl}(t), u \rangle$

Dissipation distance: $\mathcal{D}(z_1, z_2) = \int_\Omega D(x, z_1(x), z_2(x))\,\mathrm{d}x$

Background on the Energetic Formulation

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$(u,z) : [0,T] \to \mathcal{F}\times\mathcal{Z}$ 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) $\mathcal{E}(t,u(t),z(t)) + \mathrm{Diss}_{\mathcal{D}}(z;[0,t]) = \mathcal{E}(0,u_0,z_0) + \int_0^t \partial_s\mathcal{E}(\cdot,u,z)\,\mathrm{d}s$

If $\mathcal{D}(z_1,z_2) = \mathcal{R}(z_2 - z_1)$ and $\mathcal{E}(t,\cdot) : \mathcal{F}\times\mathcal{Z} \to \mathbb{R}_\infty$ convex, then

(S)&(E) $\iff \begin{cases} 0 \in \partial_u\mathcal{E}(t,u,z) & \text{elastic equilibrium} \\ 0 \in \partial\mathcal{R}(\dot{z}) + \partial_z\mathcal{E}(t,u,z) & \text{flow rule} \end{cases}$

The results obtained since 2006 fall into
four categories:

1. Modeling of Temperature-Induced Phase Transformations
2. Numerical Convergence of Space-Time Discretizations
3. Γ-Limits and Microstructures
4. Models Including Rate-Dependent Effects

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Today only 1. and 2.

For 3. and 4. see the report or the web page
`www.wias-berlin.de/research-groups/pde/projects/matheonC18.html`

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

$z : \Omega \to \mathbb{R}^{d\times d}_{0,\mathrm{sym}}$ mesoscopic transformation strain

Applied fields

$\ell_{\mathrm{appl}} \in \mathrm{C}^1([0,T],\mathcal{F}^*)$ loading

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

Energy: $\mathcal{E}(t,u,z) = \int_\Omega W(\mathbf{E}(u), z, \nabla z, \theta_{\mathrm{appl}}(t))\,\mathrm{d}x - \langle \ell_{\mathrm{appl}}(t), u\rangle$

Dissipation distance: $\mathcal{D}(z_1,z_2) = \mathcal{R}(z_2 - z_1) = \int_\Omega \rho|z_2 - z_1|\,\mathrm{d}x$

where $W = \frac{1}{2}(\mathbf{E}-z):\mathbb{C}(\theta):(\mathbf{E}-z) + H_{\mathrm{SoAu}}(z,\theta) + \sigma|\nabla z|^2$

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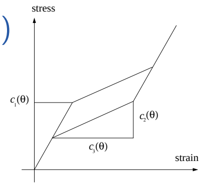
- $\mathbf{E}(u) = \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$: infinitesimal strain
- $H_{\mathrm{SoAu}}(z,\theta) = c_1(\theta)|z| + \frac{c_2(\theta)}{2}|z|^2 + \chi_{\{|z|\le c_3(\theta)\}}(z)$
  - $c_1(\theta)$: activation threshold
  - $c_2(\theta)$: hardening in the martensitic regime
  - $c_3(\theta)$: maximal transformation strain



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Regularized version of H_{SoAu}:

$H_\delta(z,\theta) = c_1(\theta)\sqrt{\delta^2+|z|^2} + \frac{c_2(\theta)}{2}|z|^2 + \frac{1}{\delta}\big(|z|-c_3((\theta))^+\big)^3$

Theorem (Existence and uniqueness)

For all $\delta \geq 0$ *there exists a solution of* ***(S)&(E)***.

For $\delta > 0$ *the solutions are unique* since $\mathcal{E} \in \mathrm{C}^3([0,T]\times\mathrm{H}^1(\Omega))$.

Finite-element spaces $\mathcal{F}_h \subset \mathcal{F}$ and $\mathcal{Z}_h \subset \mathcal{Z}$, time step $\tau > 0$

Space-Time Discretization for general systems

$$(\mathrm{IMP})^{h,\tau} \qquad (u_k^{h,\tau}, z_k^{h,\tau}) \in \underset{(u,z)\in\mathcal{F}_h\times\mathcal{Z}_h}{\mathrm{Argmin}} \Big(\mathcal{E}(k\tau, u, z) + \mathcal{D}(z_{k-1}^{h,\tau}, z)\Big)$$

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

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Theorem (Convergence of the space-time discretization)

There exists a subsequence $(\overline{u}^{h_n,\tau_n}, \overline{z}^{h_n,\tau_n})$ such that this subsequence converges to a solution (u, z) of ***(S)&(E)****.*

- Problem: solutions of **(S)&(E)** are not unique.
- uniform a priori estimates $\rightsquigarrow$ *numerical stability*
- accumulation points are solutions $\rightsquigarrow$ *consistency* (no ghost slns.)

For the regularized **Souza-Auricchio model** ($\delta > 0$) we have

- uniqueness of solutions and
- higher spatial regularity

$$(u, z) \in \mathrm{L}^\infty([0,T], \mathrm{H}^2(\Omega)) \times \mathrm{W}^{1,\infty}([0,T], \mathrm{H}^1(\Omega))$$

by studying the elliptic problem

$$\begin{cases} -\mathrm{div}\,(\mathbb{C}(\theta_{\mathrm{appl}}(t)):(\mathbf{E}(u)-z)) = \ell_{\mathrm{appl}}(t) \text{ in } \Omega \,\&\text{ bdy. cond.} \\ \mathbb{C}(\theta_{\mathrm{appl}}(t)):(z-\mathbf{E}(u)) + \mathrm{D}_z H_\delta(z, \theta_{\mathrm{appl}}(t)) - \sigma\Delta z + \underbrace{\partial\mathcal{R}(\dot{z})}_{\in \mathrm{L}^\infty(\Omega)} \ni 0 \end{cases}$$

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Theorem (Explicit convergence rates for SoAu model)

$\forall\, \delta > 0\ \exists\, C, \gamma > 0 :\ \|(u(t_k), z(t_k)) - (u_k^{\tau,h}, z_k^{\tau,h})\|_{\mathrm{H}^1} \le C(\tau^{1/2} + h^{\gamma/2})$

where $h > 0$ is the mesh size of a finite-element discretization.

Cooperations within Application Area C

- **C13:** study of incremental minimization problems
  ⇝ relaxation of non-quasiconvex problems
  ⇝ analysis of acumulated errors in many timesteps
- **C17** (just starting): efficient solution of nonsmooth minimization problems via semi-smooth Newton methods

Cooperations with ICM Warszawa

M. Danielewski, M. Gokieli, P. Rybka

External Cooperations

- **Mathematics:** G. Francfort (Paris), A. Garroni (Roma), L. Paoli (St. Etienne), T. Roubíček (Praha), U. Stefanelli (Pavia), C. Zanini (Trieste),
- **Engineering:** F. Auricchio (Pavia), S. Govindjee (Zürich), K. Hackl (Bochum), P.M. Mariano (Firenze), J.A.C. Martins (Lisboa), Ch. Miehe (Stuttgart), J. Zeman (Praha).

Plans for 2008/2009 and beyond

Outlook:

- improve the convergence rates $O(\tau^\alpha + h^\gamma)$
- find efficient solvers for $(\mathrm{IMP})^{h,\tau}$
  $\rightsquigarrow$ collaboration with **C13** and **C17**
- study polycrystalline and grain-boundary effects
  $\rightsquigarrow$ collaboration with **M. Gokieli** (ICM)
- understand the limit when $\sigma \to 0$ (formation of microstructure)
  $\rightsquigarrow$ collaboration with **L. Paoli**
- include rate-dependent effects like a heat equation
  $\rightsquigarrow$ collaboration with **T. Roubíček**
- develop the theory to include other multifunctional materials (ferroelectric materials, magnetostrictive materials)
- develop a FE simulation tool (2D and 3D)

Thank you for your attention

... more infos are under

www.wias-berlin.de/research-groups/pde/projects/matheonC18.html

Statistics I: Publications, Talks, etc.

Refereed Publications 09/2006-03/2008:	9
Submitted Articles:	5
Book Chapters and Books:	1+1
Plenary Lectures:	3
Invited Talks:	7
Offers (Prof. and similar):	0

A. Mielke:
Regularizations and relaxations of
time-continuous problems in plasticity
Project within the DFG Research Unit FOR 797
"Analysis and computation of microstructure in finite plasticity".
(one PostDoc for 3 years, plus 3 years possible).

D. Knees (with Ch. Kraus):
Modellierung von Schädigungsprozessen
Project in Wettbewerb der Leibniz-Gemeinschaft
(two PreDocs and one PostDoc for 2009-2011)

External cooperations with partners from Application Area C

. . . *with engineering groups as indicated above*

Industry projects associated with project

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Patents

—–

Statistics IV: Visibility

- A. Mielke. *Warum sind moderne Materialien schlau?* MathInside-Mathematik (nicht nur) für Schüler. Urania Berlin, March 20, 2007.
- A. Mielke. *Modeling and analysis of rate-independent processes* Lipschitz Lectures at Hausdorff Center in Bonn, 12 hours, January 8–23, 2007.