Project C18

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

DFG Research Center MATHEON
mathematics for key technologies
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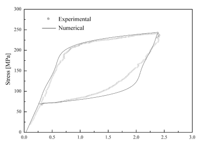
Shape-memory materials and their applications



Comparison between experiment and 1D simulation by Maletta, Falvo, Furgiuele 2007

Shape-memory materials display two special properties:

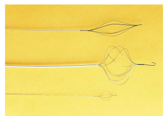
superelasticity: plateaus of almost constant stress over a large region of strains

shape memory: recovery of shape after significant deformations and subsequent thermal cycle

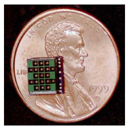
There are already many medical applications.
Currently the usage in MEMS (micro-electro-mechanical systems) is investigated.

dental wire

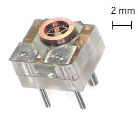
stents



baskets



microthrusters



microvalve

wires and springs

Mechanical modelling

Needs

- energetics and elastic properties of N phases **austenite** and all the variants of **martensite** (e.g.: tetragonal 1+3; orthorhombic 1+6; 1+24)
- (temperature dependent) criteria for stress and strain induced transformations

$\Longrightarrow$

Mathematical model

- **stored energy potential $\mathbf{E}$**
  $\mathbf{E}(t,\mathbf{u},\mathbf{z}) = \int_\Omega W(\nabla\mathbf{u},\mathbf{z},\theta) + \frac{\kappa}{r}|\nabla\mathbf{z}|^r \mathrm{d}x - \langle \ell(t),\mathbf{u}\rangle$
  $\mathbf{u}$ deformation, $\mathbf{z}\in\mathbb{R}^N$ phase fractions
- **dissipation potential $\mathbf{R}$**
  $\mathbf{R}(\mathbf{z},\dot{\mathbf{z}}) = \int_\Omega R(\mathbf{z}(x),\dot{\mathbf{z}}(x))\mathrm{d}x$

up to now: $\theta = \theta_{\text{applied}}(t,x)$ is prescribed as data

Subdifferential formulation of **rate-independent system** $(\mathbf{Q},\mathbf{E},\mathbf{R})$

(E) Elastic equilibrium $\quad 0 = \mathrm{D}_{\mathbf{u}}\mathbf{E}(t,\mathbf{u}(t),\mathbf{z}(t))$

(F) Phase-field equation $\quad 0 \in \partial_{\dot{\mathbf{z}}}\mathbf{R}(\mathbf{z}(t),\dot{\mathbf{z}}(t)) + \mathrm{D}_{\mathbf{z}}\mathbf{E}(t,\mathbf{u}(t),\mathbf{z}(t))$

Energetic formulation for $(\mathbf{Q},\mathbf{E},\mathbf{D})$

Weak form of **(E)&(F)** having the following advantages:

- derivative-free formulation ($\longleftarrow$ jumps, nonsmoothness)
- usage of microscopic constitutive laws for each phase $W(\cdot,e_j)$ for $j\in\{0,1,\dots,N\}$ possible
- methods from calculus of variations are available
- time-incremental problem via minimization

(IP) $\quad (\mathbf{u}_k,\mathbf{z}_k) \in \operatorname{Arg\,min}\big(\mathbf{E}(t_k,\widetilde{\mathbf{u}},\widetilde{\mathbf{z}}) + \mathbf{D}(\mathbf{z}_{k-1},\widetilde{\mathbf{z}})\big)$

Challenges

- establish existence and uniqueness for **(IP)** and for **energetic solutions** of $(\mathbf{Q},\mathbf{E},\mathbf{D})$
- numerical approximation for **(IP)** and convergence to energetic solutions (with error bounds)
- include rate-dependent effects like the heat equation
- develop the theory to include other multifunctional materials like ferroelectric materials
- develop a simulation tool for 2D and 3D models

Numerical convergence results

We use the abstract Γ-convergence theory of [MRS08] to establish convergence of numerical approximations:

Piecewise constant interpolants $(\overline{\mathbf{u}}_{\tau,h},\overline{\mathbf{z}}_{\tau,h}) : [0,T] \to \mathbf{Q}_h \subset \mathbf{Q}$

Theorem ([MR09,MPP08]) Under natural conditions $(\overline{\mathbf{u}}_{\tau_n,h_n}(t),\overline{\mathbf{z}}_{\tau_n,h_n}(t)) \to (\mathbf{u}(t),\mathbf{z}(t))$ and $(\mathbf{u},\mathbf{z})$ is an energetic solution of $(\mathbf{Q},\mathbf{E},\mathbf{D})$.

Isothermal Souza-Auricchio model (convex $\mathbf{E}$, unique solutions)

$W(\mathbf{e},\mathbf{z}) = \frac{1}{2}(\mathbf{e}-\mathbf{z}):\mathbb{C}:(\mathbf{e}-\mathbf{z}) + H_\delta(\mathbf{z})$ with hardening function

$H_\delta(\mathbf{z}) = c_1\sqrt{\delta^2+|\mathbf{z}|^2} + \frac{c_2}{2}|\mathbf{z}|^2 + \frac{1}{\delta}\big(\max\{0,|\mathbf{z}|-c_3\}\big)^3$

Theorem (see [MP*09]) For good spatial discretizations $\mathbf{Q}_h$ there exist $C>0$ and $s\in(0,1]$ such that
$\|(\overline{\mathbf{u}}_{\tau,h}(t),\overline{\mathbf{z}}_{\tau,h}(t)) - (\mathbf{u}(t),\mathbf{z}(t))\|_{\mathrm{H}^1} \le C(\tau^{1/2}+h^{s/2})$

Cooperations *inside* MATHEON: C11, C13, C17 (Hömberg-Tröltzsch, Carstensen, Kornhuber-Sprekels)
outside MATHEON:
Engrg: F. Auricchio, S. Govindjee, K. Hackl, C. Miehe, M. Ortiz
Math: M. Kružík, D. Knees, Ch. Kraus, L. Paoli, T. Roubíček, U. Stefanelli

[MRS08] A. Mielke, T. Roubìček, U. Stefanelli. Γ-limits and relaxations ... Calc. Var. PDE 31, 387-416, 2008.
[MR09] A. Mielke, T. Roubìček. Numerical approaches ... ESAIM Math. Mod. Num. Anal. 2009, to appear.
[MPP08] A. Mielke, L. Paoli, A. Petrov. On existence and approximation for 3D model of thermally-induced phase transformations in shape-memory alloys. 2008. Submitted. WIAS preprint 1330.
[MP*09] A. Mielke, L. Paoli, A. Petrov, U. Stefanelli. Error estimates for space-time discretizations of a rate-independent variational inequality. 2009. Submitted. WIAS preprint 1407.