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Project C18

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

Alexander Mielke Adrien Petrov

Weierstrass Institute for
Applied Analysis and
Stochastics

Domain of Expertise: Phase Transitions

SMA and their applications

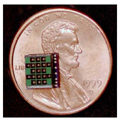
Shape-Memory Alloys (SMA) display two special properties:

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

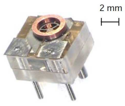
Shape memory: recovery of shape after significant deformations and subsequent thermal cycle

There are already many medical applications. Currently the usage in Micro-Electro-Mechanical Systems (MEMS) is investigated.

dental wire



mircothrusters



microvalve

wires and springs

Mechanical modelling

- Energetics and elastic properties of N phases: all the variants of **martensite** and **austenite**
- Temperature dependent criteria for stress and strain induced transformations

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

Material models are described by **generalized gradient systems** $(\mathbf{Q},\mathbf{E},\mathbf{R})$

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

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

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

Rate-Independent Systems (RIS):

$\mathbf{R}$ can be replaced by a **dissipation distance $\mathbf{D}$**

- Derivative-free formulation (← jumps, nonsmoothness)
- Usage of microscopic constitutive laws for each phase $W(\cdot,e_j)$ for $j\in\{0,1,\dots,N\}$ possible
- Time-incremental problem via minimization

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

Results

- Existence of energetic solution for thermally driven phase transformations [MP07, MPP09]
- Γ-convergence for evolutionary problems [MRS08]
- Numerical convergence

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

  for $\mathbf{E}$ general we have (see [MR09, MPP09])

$$\boxed{(\overline{\mathbf{u}}_{\tau_n,h_n}(t),\overline{\mathbf{z}}_{\tau_n,h_n}(t))\to(\mathbf{u}(t),\mathbf{z}(t))}$$

for $\mathbf{E}$ smooth and convex we have (see [MPS10])

$$\boxed{\|(\overline{\mathbf{u}}_{\tau,h}(t),\overline{\mathbf{z}}_{\tau,h}(t))-(\mathbf{u}(t),\mathbf{z}(t))\|_{\mathrm{H}^1}\leq C(\tau^{1/2}+h^{s/2})}$$

Future Goals

- Existence and uniqueness of **energetic solutions**
- Convergence of **numerical schemes**
- Inclusion of **rate-dependent effects** like heat equation
- Generalization to **other materials** like TWIP steel
- Development of a **simulation tool** for 2D and 3D

Collaborations

inside MATHEON: C11, C17, C32
Hömberg-Tröltzsch, Kornhuber-Sprekels, Knees-Kraus
outside MATHEON:
Engrg: Auricchio, Govindjee, Hackl, Miehe, Ortiz
Math: Paoli, Rossi, Roubíček, Savaré, Stefanelli

Numerics

Fig. 1

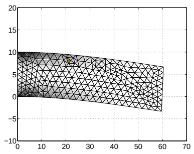


Fig. 2

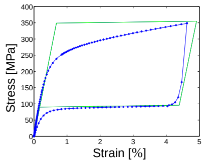


Fig. 1:Deformed mesh.

Fig. 2: Stress-strain diagrams for a loading cycle; 1D theory (green), 2D simulation (blue).

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[MR09] A. Mielke, T. Roubìček. Numerical approaches to rate-independent processes and applications in inelasticity. *ESAIM Math. Mod. Num. Anal.*, 43:399-428, 2009.
[MPP09] A. Mielke, L. Paoli, A. Petrov. On existence and approximation for 3D model of thermally-induced phase transformations in SMA. *SIAM J. Math. Anal.*, 41:1388-1414, 2009.
[MPS10] A. Mielke, L. Paoli, A. Petrov, U. Stefanelli. Error estimates for space-time discretizations of a rate-independent variational inequality. *SIAM J. Numer. Anal*, 2010. To appear.