An introduction about Shape Memory Alloys: modeling and recent mathematical results

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Workshop on Optimization, Control Theory and Applications

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Non-isothermal models

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M. E., L. Lussardi, U. Stefanelli DCDS-S (2013); **M. E., J. Kopfová, P. Krejčí** work in progress

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- Shape memory alloy (SMA)
- Shape memory effect and pseudoelasticity (martensite and austenite)
- The Souza-Auricchio model (extension with permanent inelasticity)
- Thermal control of the Souza-Auricchio model
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Shape memory alloys

- Shape memory alloys (SMAs) are examples of *active materials*: comparably large strains can be induced (activated) by means of external mechanical, thermal or magnetic stimuli
- At suitably high temperatures SMAs completely recover strains (as large as 8%) during loading-unloading cycles: this is the so called: *super-elastic* SMA behaviour
- At lower temperatures permanent deformations remain under unloading; still, the specimen can be forced to recover its original shape by heating: this is the so called *shape-memory effect*
- Finally some specific SMAs are *ferro-magnetic*: completely recoverable strains can be induced by the action of an external magnetic field

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The solid-solid transformation: austenite-martensite

- This amazing macroscopic behaviour is the result of an abrupt and diffusionless solid-solid phase transformation between different crystallographic configurations (phases): the AUSTENITE (mostly cubic, predominant at high temperature and low stresses) and the MARTENSITES (lower symmetry variants, favored at low temperature or high stresses)
- As long as it is not required a migration of the atoms, the process will only depend on the temperature and will be rate-independent
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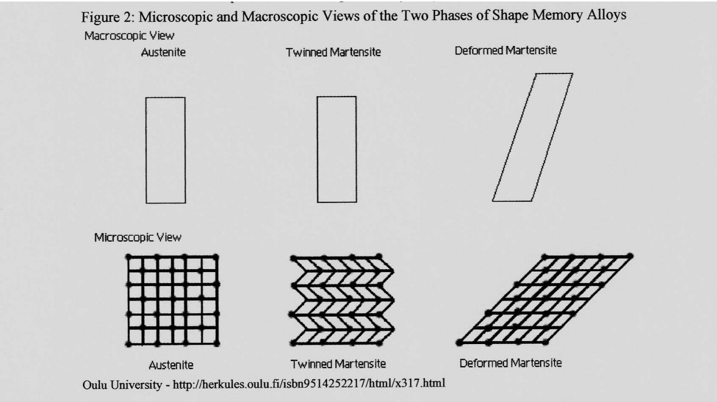

Figure 1: Macroscopic and microscopic view of the two SMA phases.

The shape memory efect

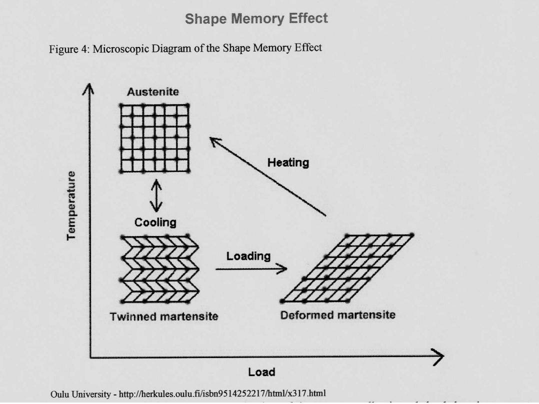

Figure 2: The shape memory effect can be obtained by cooling the alloy until it becomes totally twinned martensite. The original shape can be recovered only suitably heating the alloy; the heat transfer is the responsible for the molecular rearrangement.

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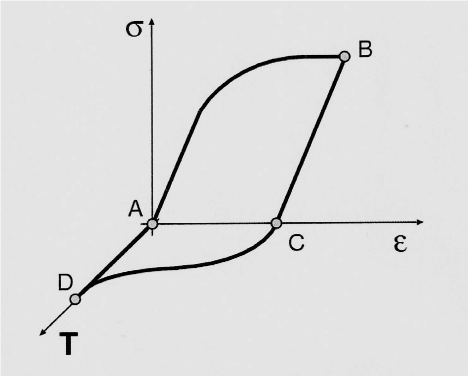

Figure 3: The shape memory effect: at the end of the loading-unloading process (ABC) at a fixed temperature, the material has a residual strain that can be recovered after a thermic cycle (CDA).

Pseudo-elasticity

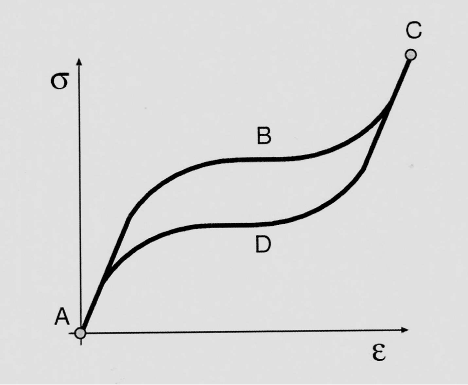

Figure 4: Pseudo-elasticity (o super-elasticity): the material loaded at a fixed temperature (ABC) shows a nonlinear behaviour. During the unloading process (CDA) we have the inverse transformation, with non-zero residual strain. Notice the *hysteresis*.

Applications

- **Mechanical and electronic engineering:** robotic actuators, micromanipulators
- **Fire security, protection systems and temperature sensors:** thermostats
- **Aeronautics:** space shuttle, hydraulic fittings for airplanes
- **Medical applications:** orthodontic wires, anchors with Nitinol hooks to attach tendons to bones, vascular stents, reinforcement for arteries and veins, vena-cava filters

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From the modelistic viewpoint

- From a modelistic viewpoint: lots of models have been proposed by addressing:
  - different alloys (NiTi among the others)
  - at different scales (atomistic, microscopic with micro-structures, mesoscopic with volume fractions, macroscopic)
  - emphasizing different principles (minimization of stored energy vs. maximization of dissipation, phenomenology vs. rational crystallography and Thermodynamics)
  - and different structures (single cristals vs. polycrystalline aggregates, possibly including intergranular interaction)
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The Souza-Auricchio model: from the mathematical viewpoint

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The Souza-Auricchio model

- We are in the regime of small deformations

$$\varepsilon = \varepsilon_{ij} = \left(\frac{u_{i,j} + u_{j,i}}{2} \right)$$

linearized strain tensor (u displacement)

- $\varepsilon = \varepsilon^{el} + \varepsilon^{tr}$ elastic and inelastic part or transformation part
- ε^{tr} at a microscopic level, describes the mechanical tensorial effect due to the deformation observed in the martensite

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The Souza-Auricchio model

- Energy density stored by the system

$$E(\varepsilon,\varepsilon^{tr}) = \frac{1}{2}\mathbb{C}(\varepsilon-\varepsilon^{tr}):(\varepsilon-\varepsilon^{tr})+c_1|\varepsilon^{tr}|+c_2|\varepsilon^{tr}|^2+I(\varepsilon^{tr})+\frac{\nu}{2}|\nabla\varepsilon^{tr}|^2$$

- the evolution of the material is described by the following classical relations (D dissipation potential)

$$\sigma = \frac{\partial E}{\partial \varepsilon}; \quad -\xi = \frac{\partial E}{\partial \varepsilon^{tr}}; \quad -\dot{\varepsilon}^{tr} = \nabla D^*(\xi)$$

- that can also be conveniently rewritten, using the instruments of the Convex Analysis, in the following subdifferential formulation

$$\begin{pmatrix} 0 \\ \partial D(\dot{\varepsilon}) \end{pmatrix} + \begin{pmatrix} \partial_{\varepsilon} E(\varepsilon,\varepsilon^{tr}) \\ \partial_{\varepsilon^{tr}} E(\varepsilon,\varepsilon^{tr}) \end{pmatrix} \ni \begin{pmatrix} \sigma \\ 0 \end{pmatrix}$$

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- The key point is the fact that the evolution of the problem can be rewritten within the so called *energetic formulation* for processes RATE-INDEPENDENT recently proposed by **A. Mielke** and co-authors
- The energetic formulation is equivalent to rewrite the problem, posed in a subdifferential form, as the sum of a **global stability** condition and a relation of **energy conservation**
- In particular the previous relations can be rewritten as:
- **Stability** $(\varepsilon(t), \varepsilon^{tr}(t)) \in \text{Arg Min}_{\bar{\varepsilon}, \bar{\varepsilon}^{tr}} (E(\bar{\varepsilon}, \bar{\varepsilon}^{tr}) - \sigma(t) : \bar{\varepsilon} + D(\bar{\varepsilon}^{tr} - \varepsilon(t)))$
- **Energy conservation**

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\begin{aligned}
& E(\varepsilon(t), \varepsilon^{tr}(t)) - \sigma(t) : \varepsilon(t) + \text{Diss}_D(\varepsilon^{tr}, [0,t]) \\
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F. Auricchio, A. Mielke, U. Stefanelli (2008)

- Analysis of the constitutive relation (without coupling with the equilibrium problem)
- The evolution problem (energetic solution + boundary conditions + $[\nabla \cdot \sigma + f = 0]$)
- Limits for $\rho \to 0$ and $\nu \to 0$

Theorem

- Existence of an energetic solution for $\rho \geq 0$
- Lipschitz continuity of solutions
- Continuous dependence of data for $\rho > 0$
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$$|(\varepsilon - \varepsilon^n)(t)| + |(\varepsilon^{tr} - \varepsilon^{tr}_n)(t)| \leq C(\tau^n)^{1/2} \ \forall t \in [0, T]$$

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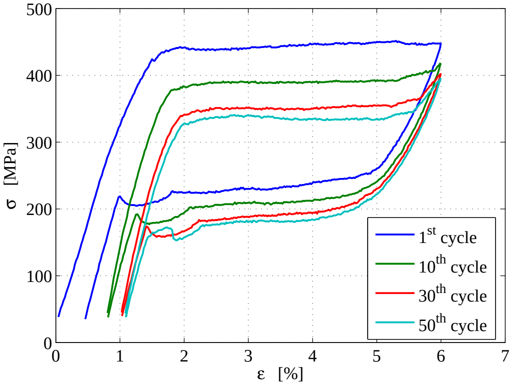
Permanent inelasticity



The Souza-Auricchio model with permanent inelasticity

Well-posedness

M. E., L. Lussardi, U. Stefanelli (2011)

- $\varepsilon = \varepsilon^{\mathrm{el}} + \varepsilon^{\mathrm{tr}} + \varepsilon^{\mathrm{pl}}$

$$E(\varepsilon, \varepsilon^{\mathrm{tr}}, \varepsilon^{\mathrm{pl}}) := \frac{1}{2}(\varepsilon - \varepsilon^{\mathrm{tr}} - \varepsilon^{\mathrm{pl}}):\mathbb{C}:(\varepsilon - \varepsilon^{\mathrm{tr}} - \varepsilon^{\mathrm{pl}}) + \alpha_T|\varepsilon^{\mathrm{tr}}| + \frac{1}{2}\varepsilon^{\mathrm{tr}}:\mathbb{H}^{\mathrm{tr}}:\varepsilon^{\mathrm{tr}} + \frac{1}{2}\varepsilon^{\mathrm{pl}}:\mathbb{H}^{\mathrm{pl}}:\varepsilon^{\mathrm{pl}} + \varepsilon^{\mathrm{tr}}:\mathbb{A}:\varepsilon^{\mathrm{pl}} + I(\varepsilon^{\mathrm{tr}} + \varepsilon^{\mathrm{pl}})$$

$$\begin{pmatrix} 0 \\ \partial_{\dot\varepsilon^{\mathrm{tr}}} D(\dot\varepsilon^{\mathrm{tr}}, \dot\varepsilon^{\mathrm{pl}}) \\ \partial_{\dot\varepsilon^{\mathrm{pl}}} D(\dot\varepsilon^{\mathrm{tr}}, \dot\varepsilon^{\mathrm{pl}}) \end{pmatrix} + \begin{pmatrix} \partial_{\varepsilon} E(\varepsilon, \varepsilon^{\mathrm{tr}}, \varepsilon^{\mathrm{pl}}) \\ \partial_{\varepsilon^{\mathrm{tr}}} E(\varepsilon, \varepsilon^{\mathrm{tr}}, \varepsilon^{\mathrm{pl}}) \\ \partial_{\varepsilon^{\mathrm{pl}}} E(\varepsilon, \varepsilon^{\mathrm{tr}}, \varepsilon^{\mathrm{pl}}) \end{pmatrix} \ni \begin{pmatrix} \sigma \\ 0 \\ 0 \end{pmatrix}$$

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The Souza-Auricchio model with permanent inelasticity

Asymptotic analysis

M. E., L. Lussardi, U. Stefanelli (2011)

- Dissipation density

$$D(\dot{\varepsilon}^{\rm tr}, \dot{\varepsilon}^{\rm pl}) = \Big((R^{\rm tr})^p |\dot{\varepsilon}^{\rm tr}|^p + (R^{\rm pl})^p |\dot{\varepsilon}^{\rm pl}|^p \Big)^{1/p}, \quad p \in [1, \infty]$$

- We are interested in dealing with the case of the limits $R^{\rm tr} \to \infty$ and $R^{\rm pl} \to \infty$ which correspond to the *purely plastic* and *purely SA* regimes respectively

- Moreover we are interested in analyzing the case $\rho \to 0$

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M. E., L. Lussardi, U. Stefanelli (2011)

- Dissipation density

$$D(\dot{\varepsilon}^{\mathrm{tr}}, \dot{\varepsilon}^{\mathrm{pl}}) = \left((R^{\mathrm{tr}})^p |\dot{\varepsilon}^{\mathrm{tr}}|^p + (R^{\mathrm{pl}})^p |\dot{\varepsilon}^{\mathrm{pl}}|^p \right)^{1/p}, \quad p \in [1, \infty]$$

- We are interested in dealing with the case of the limits $R^{\mathrm{tr}} \to \infty$ and $R^{\mathrm{pl}} \to \infty$ which correspond to the *purely plastic* and *purely SA* regimes respectively

- Moreover we are interested in analyzing the case $\rho \to 0$

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Thermal control of the Souza-Auricchio model

Thermal control of the SA model

M. E., L. Lussardi, U. Stefanelli, (2013)

Novelty of the paper

- We establish a new existence result for the problem: given the temperature, to determine the mechanical quasi-static evolution of the alloy (with less regularity requested for the temperature)
- Existence of an optimal control for a large class of cost functionals which depend both on the mechanics and the temperature

Assumptions

- We assume to be able to control the temperature in time - ok if the specimen is relatively thin in at least one direction and the loading-unloading cycles have low frequency (it is possible to assume that the heat producted is almost instantaneously dissipated)
- We assume that the temperature is spatially homogeneous in the specimen

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Thermal control of the Souza-Auricchio model

The state problem

$$
\begin{aligned}
&\mathbb{C}(\varepsilon(u) - z) = \sigma && \text{in } \Omega \times (0,T)\\
&\nabla \cdot \sigma + f = 0 && \text{in } \Omega \times (0,T)\\
&u = u^{\mathrm{Dir}} && \text{on } \Gamma_{\mathrm{Dir}} \times (0,T)\\
&\sigma n = g && \text{in } \Gamma_{\mathrm{tr}} \times (0,T)\\
&\partial \mathscr{D}(\dot{z}(t)) + \partial_z \mathscr{W}(u(t), z(t); \theta(t)) \ni 0 && \text{in } L^2(\Omega; \mathbb{R}^3_{\mathrm{dev}}),\ \forall t \in (0,T)\\
&u(0) = u^0, \qquad z(0) = z^0 && \text{in } \Omega
\end{aligned}
$$

Theorem

If $u^{\mathrm{Dir}} \in W^{1,1}(0,T;H^1(\Omega;\mathbb{R}^3))$, $f \in W^{1,1}(0,T;L^2(\Omega;\mathbb{R}^3))$, $g \in W^{1,1}(0,T;L^2(\Gamma_{\mathrm{tr}};\mathbb{R}^3))$; given $\theta \in W^{1,1}(0,T)$ and $(u^0, z^0) \in \mathscr{S}(0,\theta(0))$ there exists an energetic solution (u,z) of the state problem such that $(u,z) \in W^{1,1}(0,T;H^1(\Omega;\mathbb{R}^3) \times L^2(\Omega;\mathbb{R}^{3\times 3}_{\mathrm{dev}}))$

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An optimal control problem

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- $\mathrm{Sol}(\theta) \subset W^{1,1}(0,T;H^1(\Omega;\mathbb{R}^3) \times L^2(\Omega;\mathbb{R}^{3\times 3}_{\mathrm{dev}}))$
- minimization of the functional $\mathscr{J} : W^{1,1}(0,T;H^1(\Omega;\mathbb{R}^3) \times L^2(\Omega;\mathbb{R}^{3\times 3}_{\mathrm{dev}})) \times \Theta \to (-\infty,\infty]$
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- Example of a quadratic cost functional covered by our theory

$$J(u,z,\theta) = \int_0^T\int_\Omega |u-u_{\mathrm{d}}|^2 \,\mathrm{d}x\,\mathrm{d}t + \int_0^T\int_\Omega |z-z_{\mathrm{d}}|^2 \,\mathrm{d}x\,\mathrm{d}t + \int_\Omega |u(T)-u_{\mathrm{f}}|^2 \,\mathrm{d}x + \int_\Omega |z(T)-z_{\mathrm{f}}|^2 \,\mathrm{d}x$$

$u_{\mathrm{d}} : [0,T] \to L^2(\Omega;\mathbb{R}^d)$, $z_{\mathrm{d}} : [0,T] \to L^2(\Omega;\mathbb{R}^{d\times d})$ given preferred displacement and inelastic strain profiles $u_{\mathrm{f}} \in L^2(\Omega;\mathbb{R}^d)$ and $z_{\mathrm{f}} \in L^2(\Omega;\mathbb{R}^{d\times d})$ given target states

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Thermal control of the Souza-Auricchio model

In order to possibly find optimal controls we shall consider the following standard requirements

Compatibility of the initial value and the controls:

$(u^0, z^0) \in \mathscr{S}(0, \theta(0)) \quad \forall \theta \in \Theta$

Compactness of controls:

Θ is weakly compact in $W^{1,r}(0,T)$ for some $r > 1$

Lower semicontinuity of the cost functional:

$$\left.\begin{array}{l} \theta_n \to \theta \text{ weakly in } W^{1,r}(0,T) \\ (u_n, z_n) \in \mathrm{Sol}(\theta_n), \\ (u_n, z_n) \to (u, z) \text{ weakly-star in} \\ L^\infty(0,T; H^1(\Omega;\mathbb{R}^d) \times L^2(\Omega;\mathbb{R}^{3\times3}_{\mathrm{dev}})) \end{array}\right\} \Rightarrow \mathscr{J}(u, z, \theta) \le \liminf_{n\to\infty} \mathscr{J}(u_n, z_n, \theta_n)$$

A problem of thermodynamical consistency

Focus on the non-isothermal case

P. Krejčí, U. Stefanelli, (2011)

The state of the art

- The isothermal case: *given and uniform temperature*. The only behaviour analyzed is the super-elastic (or pseudo-elastic) regime
- The *temperature is assumed to change in time* but still is *a priori given.* Justification... However the experimental data on wires reveal that the heat production due to dissipation for the phase transformation is not negligible

Content of the paper

- Analysis of the complete quasi-static thermomechanical evolution of the specimen described by the SA model; the *temperature is an unknown of the system*
- Main result: existence for the system of nonlinear PDEs which derive from constitutive relations, conservation of momentum and energy

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Crucial point

- To give a constructive proof of the fact that the original formulation of the SA model necessarily requires some *(small) modifications* in order to BE THERMODYNAMICALLY CONSISTENT (modifications which are compatible with the experimental data)
- In particular it is proved that the model is ill-posed if the dependence of the latent heat from the temperature is not smooth enough or if the hardening constant is too small or if the dissipation is too big. In all these cases explicit solutions are constructed for which the existence fails for all times

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A new approach

The temperature dependent Preisach model

M. E., J. Kopfová, P. Krejčí work in progress

1D stress-strain relation

$$\varepsilon = \frac{\sigma}{E} + \varepsilon_L Q\left(\frac{1}{E_h \varepsilon_L}\mathfrak{p}_r[\sigma - f(\theta)]\right)$$

$$\Updownarrow$$

$$\sigma = E\varepsilon - E\varepsilon_L Q\left(\frac{E}{(E_h + E)\varepsilon_L}\mathfrak{p}_{r/E}\left[\varepsilon - \frac{f(\theta)}{E}\right]\right),$$

The play operator

$$|v(t) - \xi_r(t)| \le r \quad \forall t \in [0,T];$$
$$\dot{\xi}_r(t)(v(t) - \xi_r(t) - y) \ge 0 \quad \text{a.e.} \quad \forall |y| \le r\,.$$

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Our proposal

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Regularization inspired on the Preisach model

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Our proposal

Advantages: it is consistent from the thermodynamic viewpoint
But: more complicated with respect to the original SA model
Main aim: well posedness of the whole dynamical system and thermodynamical consistency

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