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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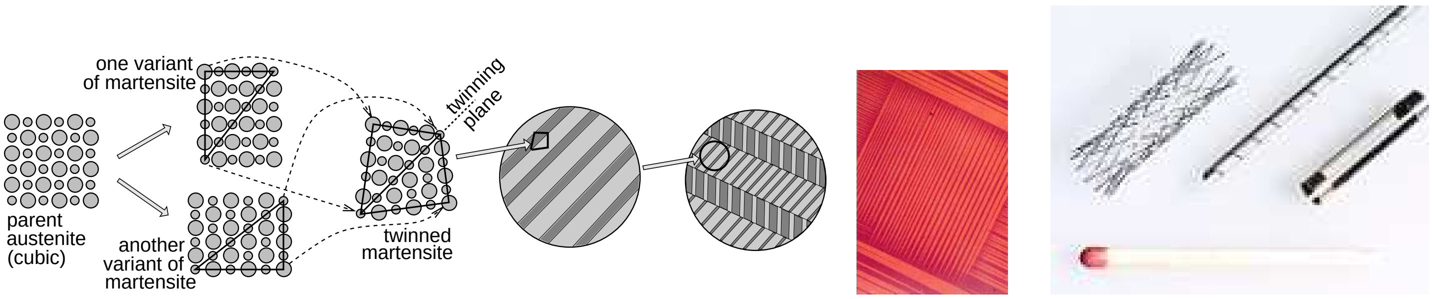
Multiscale modelling in shape-memory materials



atomistic scale   micro-scale   meso-scale   macro-scale

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

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

Energetic formulation of rate-independent evolution via (S) and (E) (see [Mie07])

(S) static stability $\quad \mathbf{E}(t,\varphi(t),z(t))\le \mathbf{E}(t,\widetilde\varphi,\widetilde z)+\mathbf{D}(z(t),\widetilde z)$ for all $\widetilde\varphi,\widetilde z$

(E) energy balance $\quad \mathbf{E}(t,\varphi(t),z(t))+\int_0^t \mathbf{R}(z(s),\dot z(s))\,\mathrm{d}s=\mathbf{E}(0,\varphi(0),z(0))+\int_0^t \partial_s\mathbf{E}(s,\varphi(s),z(s))\,\mathrm{d}s$

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) $\quad (\varphi_k,z_k)\in \operatorname{Arg\,min}\mathbf{E}(t_k,\widetilde\varphi,\widetilde z)+\mathbf{D}(z_{k-1},\widetilde z)$

Challenges

- establish existence and uniqueness for **(IP)** and for **(S)&(E)**
- study the influence of interfacial energy and the Γ-limit for vanishing interfacial energy
- numerical approximation for **(IP)** and convergence to **(S)&(E)** with optimal rates
- include proper heat equation

Souza-Auricchio model

- **State variables and applied fields**
  $\varphi:\Omega\to\mathbb{R}^d$ displacement $\left(e(\varphi)=\frac12(\nabla\varphi+\nabla\varphi^T)\right)$
  $z:\Omega\to\mathbb{R}^{d\times d}_{0,\text{sym}}$ mesoscopic transformation strain
  $l\in C^1([0,T];H^{-1}(\Omega))$ exterior loading
  $\theta=\theta_{\text{appl}}\in C^1([0,T];L^\infty(\Omega))$ temperature
- **Energy and dissipation potentials**
  $W(\nabla\varphi,z,\theta)=\frac12(e(\varphi)-z){:}\mathbb{C}(\theta){:}(e(\varphi)-z)+h_\delta(z,\theta)$
  $R(z,\dot z)=\rho|\dot z|_1$

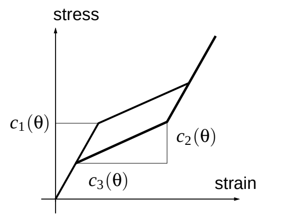
Hardening function with $\delta\in[0,1]$

$$h_\delta(z,\theta)=c_1(\theta)\sqrt{\delta^2+|z|^2}+\frac{c_2(\theta)}{2}|z|^2+\frac{1}{\delta}\left(\max\{0,|z|-c_3(\theta)\}\right)^3$$

Theorem (see [MP07])

For all $\delta\ge 0$, **(S)&(E)** has a solution $(\varphi,z)\in C^{\text{Lip}}([0,T];H^1(\Omega;\mathbb{R}^d)\times H^1(\Omega;\mathbb{R}^{d\times d}_{0,\text{sym}}))$.

For $\delta>0$ we have $\mathbf{E}\in C^{2,\text{Lip}}([0,T];H^1(\Omega))$ and the solutions are unique.



$c_1(\theta)$ activation threshold
$c_2(\theta)$ hardening
$c_3(\theta)$ maximal transformation strain

Cooperations *inside* MATHEON: C10, C11, **C13**, C14, C15, C16 (Wagner-Münch, Hömberg, Carstenen, Niethammer-Dreyer, Melcher, Bartels)

- *in Engineering:* F. Auricchio, S. Govindjee, K. Hackl, C. Miehe, M. Ortiz
- *in Mathematics:* M. Kužík, L. Paoli, T. Roubíček, U. Stefanelli

[Mie07] A. Mielke: A model for temperature-induced phase transformations in finite-strain elasticity. *IMA J. Applied Math.*, 2007. To appear (WIAS preprint No 1184).

[MP07] A. Mielke, A. Petrov: Thermally driven phase transformation in shape-memory alloys. In preparation, 2007.