Modeling of multifunctional materials

how to describe evolving microstructures in solids

Alexander Mielke

Weierstraß–Institut für Angewandte Analysis und Stochastik

DFG Research Center MATHEON
Mathematics for key technologies

WIAS
Weierstraß-Institut für Angewandte Analysis und Stochastik

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Albert Einstein:

Theory determines what is observable.

Mathematical theory determines what can be calculated numerically.

Analysis substantially enlarges the class of problems that can be simulated efficiently.

Mathematical Fields	I	II	III
Application Area	Optimiz. discr.math.	Numerics sci.comp.	Applied & stoch.anal.
A Life sciences			■
B Logistics, traffic, telecomm.			
C **Production**		■	■
D Circuit sim., opto-electronics			■
E Finance			
F Visualization			
G Education, Outreach, Adm.			

Intersection of **Numerical and Applied Analysis**
and **Multifunctional Materials**

1. Multi-functional materials

Multi-functional materials combine several properties like

- elastic deformation
- magnetization
- polarization
- phase transformations
- electric and electronic properties

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Example 1:
piezo-electric effect = nontrivial coupling between
elastic deformation and polarization
$\rightsquigarrow$ use as actuator or sensors

Multi-functional materials combine several properties like

- elastic deformation
- magnetization
- polarization
- phase transformations
- electric and electronic properties

Example 2:
shape-memory effect = nontrivial coupling between
elastic deformation and phase transformation

Microstructure in multi-functional materials

The multi-functional behavior is often generated by **internal microstructure**

e.g., in **wood**

- elasticity
- inflammability
- heat insulation
- water sensitivity

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Steel

outside hard and inside soft

Excalibur

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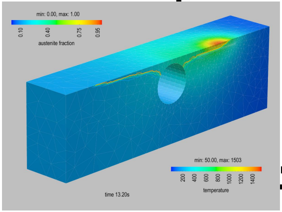
Steel

outside hard and inside soft

C11 Modeling and optimization of phase transitions in steel



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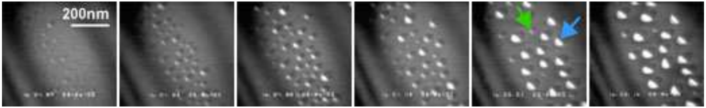
C10 Thin-film nanostructures on crystal surfaces



quantum dots

C14 Macroscopic models for precipitation in crystalline solids

Shape-memory effect

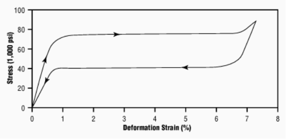
drastic permanent deformation

$\rightsquigarrow$ heating

$\rightsquigarrow$ material remembers original shape

Super-elasticity

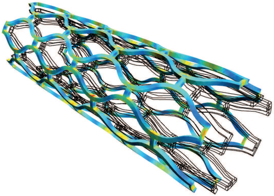
Nickel-**Ti**tan **N**ational **O**rdinace **L**aboratory 1961 Nitinol



- large plateau (constant stresses)
- hysteresis loop (energy absorption)

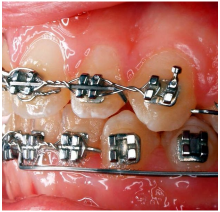
Applications of the super-elastic effect in medicine:

stents for blood vessels

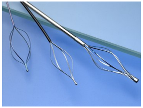
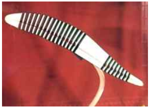
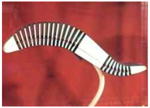


separators

dental braces



2. Shape-memory alloys

-  Medical grippers without joints
- Deformable airplane wings  
- MEMS micro-electronical-mechanical systems
  micro-gripper, -pumps, -valves
  (without any joint, screw or other disturbing part)

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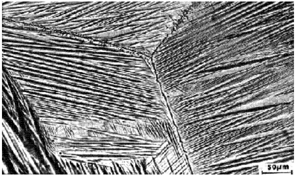
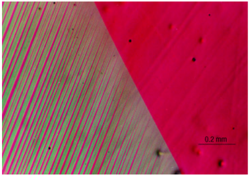
2. Shape-memory alloys: microstructure

These effects rely on microstructural arrangements of different phases

CuAlNi alloy
(Hornbogen, Bochum)





NiMaGa alloy

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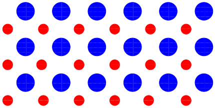
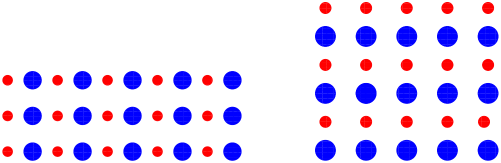
right: austenite
left: twinned martensite
(Chu, James)

austenite = symmetric high-temperature phase
martensite = less symmetric, low temperature phase (several variants)

2. Shape-memory alloys: microstructure

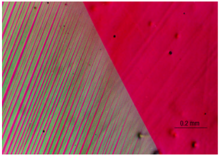




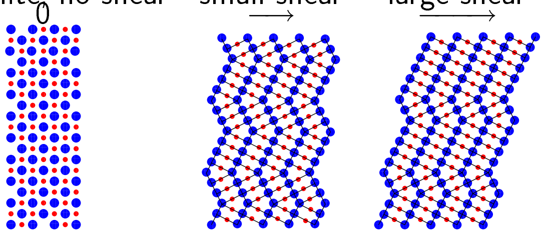
symmetric, high-temperature
low stresses
Austenite
Sir W.C. Roberts-Austen (1843–1902)

less symmetric, low temperature
higher stresses
two variants of **Martensite**
Adolf Martens (1850–1914)

Twinning: layering of two variants of martensite



Austenite, no shear   small shear $\longrightarrow$ large shear $\longrightarrow$



$\longleftarrow$ martensite layer

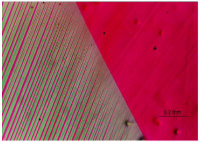
$\longleftarrow$ martensite layer

Super-elastic plateau: Easy flipping between the martensite variants.

Shape-memory effect: After heating pure austenite is produced, which returns into the original shape.

After cooling regularly layered twins reappear while keeping the shape.

Typical size of specimens: 1 mm to 1 cm
Typical size of microstructure: 100 nm to 10 μm



Numerical resolution of microstructure via Finite-Element Methods impossible or undesirable ($\geq 1000^3$ elements)

The important quantity is $\boldsymbol{F} = \nabla\phi \in \mathbb{R}^{3\times 3}$, the deformation gradient, which fluctuates wildly on the (sub-)micron scale

Idea of Ball & James 1987:

Microstructure can be described by a probability distribution:

Gradient Young measure at point $x \in \Omega$

$$\mu_x(A) \approx \frac{\mathrm{vol}(\{\, y \in B_r(x) \mid \boldsymbol{F}(y) \in A \,\})}{\mathrm{vol}(B_r(x))} \qquad \rightsquigarrow \mu_x \in \mathrm{Prob}(\mathbb{R}^{3\times 3})$$

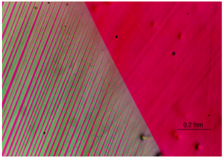
3. Mathematical modeling

Characterization of gradient Young measures ($\sim$ 1995)

- is possible via quasiconvex functions (difficult, still incomplete)
- laminates (= twins) and sequential laminates are GYMs

If $\phi : \Omega \to \mathbb{R}^3$ Lipschitz and $\nabla\phi(x) \in \{\boldsymbol{F}_1, \boldsymbol{F}_2\}$,
then $\boldsymbol{F}_1 - \boldsymbol{F}_2 = \boldsymbol{a} \otimes \boldsymbol{b}$ (rank-one matrix)

$$\left|\begin{array}{c|c|c|c|c|c|c|c} \lambda & 1-\lambda & \lambda & 1-\lambda & \lambda & 1-\lambda & \lambda & 1-\lambda \\ \boldsymbol{F}_1 & \boldsymbol{F}_2 & \boldsymbol{F}_1 & \boldsymbol{F}_2 & \boldsymbol{F}_1 & \boldsymbol{F}_2 & \boldsymbol{F}_1 & \boldsymbol{F}_2 \end{array}\right|$$



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λ	$1-\lambda$	λ	$1-\lambda$	λ	$1-\lambda$	λ	$1-\lambda$
$\boldsymbol{F}_1$	$\boldsymbol{F}_2$	$\boldsymbol{F}_1$	$\boldsymbol{F}_2$	$\boldsymbol{F}_1$	$\boldsymbol{F}_2$	$\boldsymbol{F}_1$	$\boldsymbol{F}_2$

$$\mu_x = \lambda\delta_{\boldsymbol{F}_1} + (1-\lambda)\delta_{\boldsymbol{F}_2}$$

Gradients $\boldsymbol{F} \in \mathbb{R}^{3\times 3}$ lie in a 9-dimensional linear space

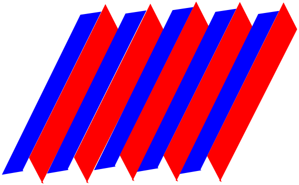
Simple laminates lie in a nonlinear 15-dimensional manifold
[$\boldsymbol{F}_1, \boldsymbol{F}_2 \in \mathbb{R}^{3\times 3}$ with $\mathrm{rank}(\boldsymbol{F}_1 - \boldsymbol{F}_2) = 1$ and $\lambda \in (0,1)$]

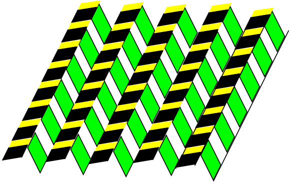
Sequential laminates

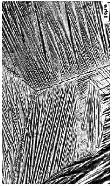
(F_1, F_2) laminate with average $F = \lambda F_1 + (1-\lambda) F_2$

Each gradient is split again into a laminate:

$$F_j = \lambda_j F_{j,1} + (1-\lambda_j) F_{j,2}, \ \mathrm{rank}(F_{j,2} - F_{j,1}) = 1, \ \lambda_j \in [0,1]$$







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Double laminates lie in a nonlinear manifold of dimension

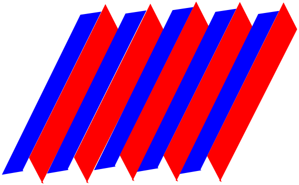
$$= 9+6+(6+6) = 27$$

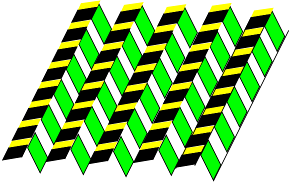
Sequential laminates

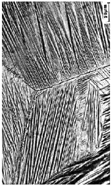
$(\boldsymbol{F}_1, \boldsymbol{F}_2)$ laminate with average $\boldsymbol{F} = \lambda \boldsymbol{F}_1 + (1-\lambda)\boldsymbol{F}_2$

Each gradient is split again into a laminate:

$$\boldsymbol{F}_j = \lambda_j \boldsymbol{F}_{j,1} + (1-\lambda_j)\boldsymbol{F}_{j,2},\ \text{rank}(\boldsymbol{F}_{j,2}-\boldsymbol{F}_{j,1}) = 1,\ \lambda_j \in [0,1]$$







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Instead of linear 100^3 unknowns in FEM for microstructure one can use 27 nonlinear unknowns obtained from analysis.

For each pure phase $e_j \in Z_{\text{pure}} = \{e_1, ..., e_N\} \subset \mathbb{R}^N$
there is given a stored-energy density $W(\boldsymbol{F}, e_j)$.
$Z = \mathrm{conv}(Z_\mathsf{p})$ Gibbs simplex of possible mixtures of phases

Mixture function $\mathbb{W} : \mathbb{R}^{3\times3} \times Z \to \mathbb{R}$ [M.&Theil'02]
(also called free-energy of mixing by Govindjee&Hackl'07)

$$\mathbb{W}(\boldsymbol{F}, z) = \min \int_{\mathbb{R}^{3\times3}\times Z_\mathsf{p}} W(\boldsymbol{G}, \widetilde{z})\, \mu(\mathrm{d}\boldsymbol{G}, \mathrm{d}\widetilde{z})$$

over $\mu \in \mathrm{Prob}^{\mathrm{GYM}}(\mathbb{R}^{3\times3}\times Z_\mathsf{p})$ with $\int_{\mathbb{R}^{3\times3}\times Z_\mathsf{p}} (\boldsymbol{G}, \widetilde{z})\mu(\mathrm{d}\boldsymbol{G}, \mathrm{d}\widetilde{z}) = (\boldsymbol{F}, z)$

$\mathbb{W}$ must be evaluated numerically using laminates or FEM, see
MATHEON C13: Adaptive simul. of PT in solid mech. (C. Carstensen) or
Institute of Fundamental Technol. Research, Polish Acad. Sci., Warszawa
H. Petryk, S. Stupkiewicz

Statics is quite well understood:

- using calculus of variations (Weierstraß' priniple)
- energy minimizers
- starting from Ball&James there are now more than 1000 papers

What about models for evolution of microstructure ?

State $q = (\phi, z) \in \mathcal{Q} = \mathcal{F} \times \mathcal{Z}$ state space

Energy storage functional
$\mathcal{E}(t, \phi, z) = \int_\Omega \mathbb{W}(x, \nabla\phi(x), z(x)) + \rho|\nabla z(x)|^\alpha \,\mathrm{d}x - \langle \ell(t), \phi \rangle$

Dissipation distance
$\mathcal{D}(z_{\mathrm{old}}, z_{\mathrm{new}}) = \int_\Omega D(x, z_{\mathrm{old}}(x), z_{\mathrm{new}}(x)) \,\mathrm{d}x$

Energetic formulation for rate-independent systems.
A function $q : [0, T] \to \mathcal{Q}$ is called *energetic solution*, if for all $t \in [0, T]$ **global stability (S)** and **energy balance (E)** hold:

(S) $\quad \mathcal{E}(t, q(t)) \leq \mathcal{E}(t, \widehat{q}) + \mathcal{D}(q(t), \widehat{q})$ for all $\widehat{q} \in \mathcal{Q}$;

(E) $\quad \mathcal{E}(t, q(t)) + \mathrm{Diss}_{\mathcal{D}}(q, [0, t]) = \mathcal{E}(0, q(0)) + \int_0^t \partial_s \mathcal{E}(s, q(s)) \,\mathrm{d}s.$

Existence theory developed in C18 by M&Petrov and coworkers.

Joint work with **Kručík & Roubíček** [Meccanica'05, M2AN'08]:

CuAlNi with cubic-to-orthorhombic phase transformation

$W_j(\boldsymbol{F}) = \frac{1}{2}(\boldsymbol{F}^\top\boldsymbol{F}-\boldsymbol{U}_j):\mathbb{C}_j:(\boldsymbol{F}^\top\boldsymbol{F}-\boldsymbol{U}_j) + \gamma_j \quad (j = 1, ..., 7)$

with experimental values for $\gamma_j, \boldsymbol{U}_j, \mathbb{C}_j$ from experiments by Šittner

Problem: mixture function $\mathbb{W}$ is not known.

Go back and use gradient Young measures!!

Joint work with **Kručík & Roubíček** [Meccanica'05, M2AN'08]:

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State space $\mathcal{Q}$ involving **gradient Young measures**:
Mesoscopic phase indicator $z = \Lambda(\boldsymbol{F})$ with continuous $\Lambda : \mathbb{R}^{3\times3} \to Z$

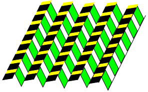
$$\widehat{\mathcal{Q}} = \Big\{(\phi,\mu,z) \in \mathrm{W}^{1,4}(\Omega)\times\mathrm{GYM}^4(\Omega;\mathbb{R}^{3\times3})\times\mathrm{L}^1(\Omega) \;\Big|\; \nabla\phi = \mathrm{id}\bullet\mu,\, z = \Lambda\bullet\mu \text{ a.e.} \Big\}$$

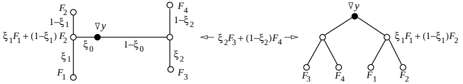
where $(\Phi\bullet\mu)(x) = \int_{\mathbb{R}^{3\times3}} \Phi(x,\boldsymbol{F})\mu(x,\mathrm{d}\boldsymbol{F})$

$$\widehat{\mathcal{E}}(t,q) = \int_\Omega (W\bullet\mu)(x) + \rho|\nabla z|^\alpha\,\mathrm{d}x - \langle \ell(t),\phi\rangle$$

Existence of energetic solutions for $(\widehat{\mathcal{Q}},\widehat{\mathcal{E}},\mathcal{D})$ can be shown.

- time discretization $0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T$
- triangulation $\mathcal{T}_h$ of domain $\Omega \subset \mathbb{R}^3$
- lamination level $\kappa = 2$ (double laminates)





Numerical phase space $\mathcal{Q}_{h,\kappa}$

$$\mathcal{Q}_{h,\kappa} = \Big\{ (\phi, \mu, z) \in \mathrm{W}^{1,4}(\Omega) \times \mathrm{GYM}^4_{\mathrm{lam},\kappa}(\Omega; \mathbb{R}^{3\times 3}) \times \mathrm{L}^1(\Omega) \;\Big|\; \nabla\phi = \mathrm{id}\bullet\mu,\ \cancel{z = \Lambda\bullet\mu},\ \mu, z \text{ pw. const. on } \mathcal{T}_h \Big\}$$

Penalized energy

$$\mathcal{E}_\delta(t, q) = \int_\Omega \Big((W\bullet\mu)(x) + \rho|\nabla z|^\alpha \Big)\,\mathrm{d}x + \frac{1}{\delta}\|\Lambda\bullet\mu - z\|^2_{\mathrm{H}^{-1}(\Omega)} - \langle \ell(t), \phi\rangle$$

Dissipation $\mathcal{D}$ as above

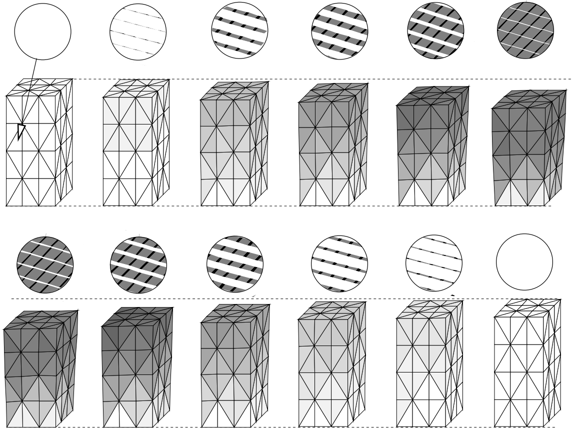
Discrete time-incremental minimization problems
$j = 1, ..., N$: $q_{h,j,\delta} \in \mathrm{Argmin}\{\, \mathcal{E}_\delta(t_j, q) + \mathcal{D}(q_{h,j-1,\delta}, q) \mid q \in \mathcal{Q}_{h,\kappa} \,\}$

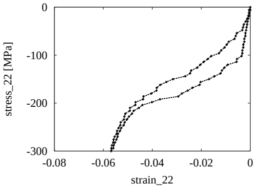
For $\max\{\, t_j - t_{j-1} \mid k = 1, ..., N \,\} \to 0$, $\delta, h \to 0$ with $h \in (0, H(\delta)]$

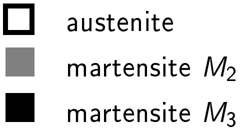
- we have uniform a priori bounds,
- we find limit points in the associated weak topologies,
- a general abstract Γ-convergence theorem is applicable.

Theorem (M&Roubíček&Stefanelli'07/'08):
Numerics converges to an energetic solution $(\widehat{\mathcal{Q}}, \widehat{\mathcal{E}}, \mathcal{D})$
(after choosing subsequences, due to non-uniqueness)

Numerical example: cyclic compression test







We see nontrivial hysteresis through sesqui-laminates:
Austenite is laminated with twinned (M_2, M_3).

Conclusions

- Analytical multiscale modeling leads to well-posed mesoscopic models.
- A dramatic reduction of unknowns is possible by giving up the linear FE structure.

- Applied analysis can identify new mesoscopic quantities, which
  - behave well in the upscaling procedure and
  - faithfully describe the effects of the microstructure.
- Nonlinear analysis may contribute substantially to the progress in simulation of complex systems.

Thank you for your attention !

Papers online under `www.wias-berlin.de/people/mielke`