Numerical Simulation of the Stress-Strain Behavior of Ni-Mn-Ga Shape Memory Alloys

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joint work with T. Roubíček and P. Šittner

Overview

I. Modeling
- Modeling on various length scales
- Elastic energy
- Dissipation
- Evolution equations

II. Numerical Implementation
- Discretization
- Solution method

III. Experimental and Numerical Results

Comparison of laboratory experiments and numerical simulations:
- Evolution of microstructure
- Stress-strain behavior

Modeling of crystalline solids on various length scales:

- Quantum mechanical level
  - Electron densities
  - Schrödinger equation and its approximations
- Atomic level
  - Atom positions, potential function
  - Newton´s equations
- Continuum mechanical level
  - Deformation function $y : \Omega \to \mathbb{R}^3$
  - Potential function, evolution equation
  - Includes „mesoscopical“ models (cf. Young measures, ...)

Multi-Scale Modeling

Interesting points:

- Upscaling (Derivation of coarse scale models from fine scale models)
  - Thermodynamic limit (Blanc, Le Bris, P.L. Lions 2002)
  - Direct expansion technique (Kruskal, Zabusky 1964, Collins 1981, Rosenau 1986)
  - Inner expansion technique (A., Griebel 2004)
  - Quasi-continuum method (Tadmor, Ortiz, Phillips 1996)

- Coupling of different models within one simulation
  - Bridging Scales Method (W. K. Liu et. al 2003)
  - Heterogeneous Multiscale Method (W. E et. al 2003)

- Analytical Methods:
  - Γ-Limit (Braides et. al 2000)
  - Many other contributions (Friesecke, Theil, Dreyer, ...)

Here:
Modeling of a Ni-Mn-Ga shape memory alloy (SMA) on the continuum mechanical level.

(Precisely: Ni-29.1wt.%Mn-21.2wt.%Ga single crystal)

Description of crystal behavior in terms of energetics:

- Elastic energy
  - Multiwell character: different phases, variants
  - Temperature dependence
- Dissipation
  - Hysteretic behavior
  - Rate independent mechanism
- Higher order contributions
  - Capillarity
  - Viscosity

→ not discussed today

Modeling of elastic energy:

- Austenite strain tensor:

$$\varepsilon^0 = \frac{1}{2}\left(\nabla y^T \nabla y - I\right)$$

- Martensite strain tensor:

$$\varepsilon^\alpha = \frac{1}{2}\left(W_\alpha^{-T} \nabla y^T \nabla y W_\alpha^{-1} - I\right)$$

- Ni-Mn-Ga undergoes cubic to tetragonal transformation. Wells for austenitic phase and martensitic variants:

$$W_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad W_1 = \begin{pmatrix} \eta_2 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix}$$

$$W_2 = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix} \quad W_3 = \begin{pmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_2 \end{pmatrix}$$

$$\eta_1 = a_M/a_0 = 1.018$$
$$\eta_2 = c_M/a_0 = 0.961$$

$$a_0 = 5.839\text{Å}$$
$$a_M = 5.945\text{Å}$$
$$c_M = 5.610\text{Å}$$

Modeling: Elastic Energy

- Quadratic form of elastic energy density for each austenite/martensite variant α:

$$\varphi_\alpha(\nabla y) = \frac{1}{2} \sum_{i,j,k,l=1}^{3} \mathbb{C}^\alpha_{ijkl} \varepsilon^\alpha_{ij} \varepsilon^\alpha_{kl}$$

- Overall elastic energy:

$$V_{\mathrm{el}}(y,\theta) = \int_\Omega \varphi(\nabla y(x),\theta)\,\mathrm{d}x$$

$$= \int_\Omega \min_{\alpha=0,\dots,3} \left(\varphi_\alpha(\nabla y(x)) + \psi_\alpha(\theta)\right)\,\mathrm{d}x$$

- Temperature-dependent offset:

$$\psi_{1,2,3}(\theta) = C(\theta - \theta_{\mathrm{eq}})$$

$$\psi_0(\theta) = 0$$

C=Clausius-Clapeyron slope

θ_{eq}=equilibrium temperature

- Elastic stress tensor: $\sigma_{\mathrm{el}} = \dfrac{\partial}{\partial \nabla y}\varphi(\nabla y,\theta)$

Modeling of dissipation:

- Obervation:
  - SMAs dissipate a certain amount of energy during each phase transformation.
  - This dissipation is (mostly) rate-independent.

→ Capture this behavior within our model.

- Introduce phase indicator functions

$$\lambda_\alpha : \mathbb{R}^{3\times 3} \to \mathbb{R}$$

for each variant α=0,1,2,3, which fulfill

- λ_α=1 nearby of well W_α
- λ_α=0 far away from well W_α
- smoothly interpolated

- Introduce dissipation potential:

$$\xi : \mathbb{R}^4 \to \mathbb{R} \qquad \xi(z) = \sum_{\alpha=0}^{3} \mathcal{E}_\alpha |z_\alpha|$$

constants describing the amount of dissipation

- Dissipation rate:

$$\xi\left(\frac{\partial}{\partial t}\lambda(\nabla y)\right)$$

- Dissipated energy over time interval $[t_1,t_2]$:

$$\xi\left(\operatorname*{Var}_{[t_1,t_2]} \lambda(\nabla y)\right)$$

(Note: total variation is a rate-independent quantity!)

- Associated quasiplastic stress tensor:

$$\sigma_{\mathrm{pl}} \in \partial\xi\left(\frac{\partial}{\partial t}\lambda(\nabla y)\right) \cdot \lambda'(\nabla y)$$

- Putting it together: Evolution equation

$$\rho \frac{\partial^2 y}{\partial t^2} = \operatorname{div}\left(\sigma_{\mathrm{el}}(\nabla y) + \sigma_{\mathrm{pl}}(\nabla y, \frac{\partial}{\partial t}\nabla y)\right)$$

ρ = mass density

- Transformation process in SMA experiments here is very slow
  → Mass density ρ can be neglected.

$$0 = \operatorname{div}\left(\sigma_{\mathrm{el}}(\nabla y) + \sigma_{\mathrm{pl}}(\nabla y, \frac{\partial}{\partial t}\nabla y)\right)$$

Initial conditions:

- Prescribe deformation and velocity at t=0

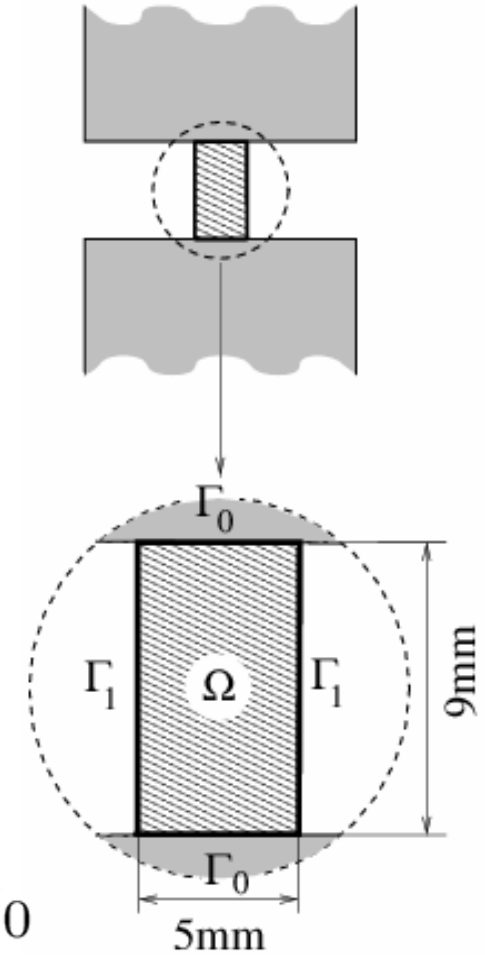
Boundary conditions:

- Time-dependent Dirichlet boundary conditions at fixed boundary part Γ_0:

$$y(x,t) = y_0(x,t), \quad x \in \Gamma_0 \subset \partial\Omega$$

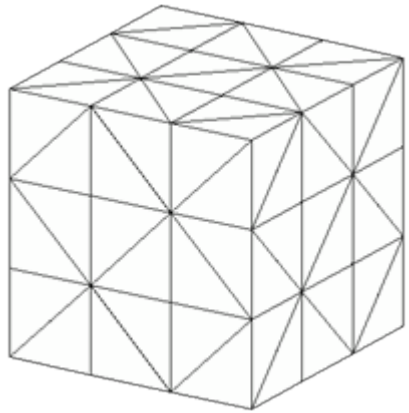
- Homogeneous Neumann boundary conditions at free boundary part Γ_1:

$$\nabla y(x,t) \cdot \nu = 0, \quad x \in \Gamma_1 = \partial\Omega \setminus \Gamma_0$$



Part II: Numerical Implementation

Goal: Solve evolution equation numerically.



Discretization in space:

- Decomposition of domain Ω into tetrahedra
- Finite Element method with P1 Lagrange ansatz functions:
  - piecewise linear on each tetrahedron
  - continuous on whole domain Ω

Discretization in time:

- Subdivide time interval into time slices:

$$0 = t_0 < t_1 < t_2 < \ldots < t_{J-1} < t_J$$

- Finite Difference method

Solution procedure:

At each time step t_j find $y^{(j)}$ which minimizes the energy functional

$$V(y^{(j)}) = V_{\mathrm{el}}(y^{(j)}) + \xi \left(\lambda(\nabla y^{(j)}) - \lambda(\nabla y^{(j-1)}) \right)$$

Theorem: Each (local) minimizer is a solution of the discretized evolution equation.

Minimization algorithm: Gradient method.

At each time step j:

- Line search: find minimum along line

$$y^{(j-1)} - s^{(j)} \nabla V(y^{(j-1)}), \qquad s^{(j)} \in \mathbb{R}$$

- Determination of step size $s^{(j)}$ by modified Armijo method:

$$\begin{aligned} s^{(j)} = & s^{(j-1)} \max\{2^i : i \in \mathbb{Z} \text{ and } \forall k \in [\min(0,i), i] \cap \mathbb{Z} : \\ & V\left(y^{(j-1)} - 2^k s^{(j-1)} \nabla V(y^{(j-1)})\right) \\ & \leq V(y^{(j-1)}) - \beta 2^k s^{(j-1)} \|\nabla V(y^{(j-1)}))\|^2 \end{aligned}$$

- Repeat this several times

Gradient method is a local minimization technique.
Improve minimization algorithm to find better minimum:

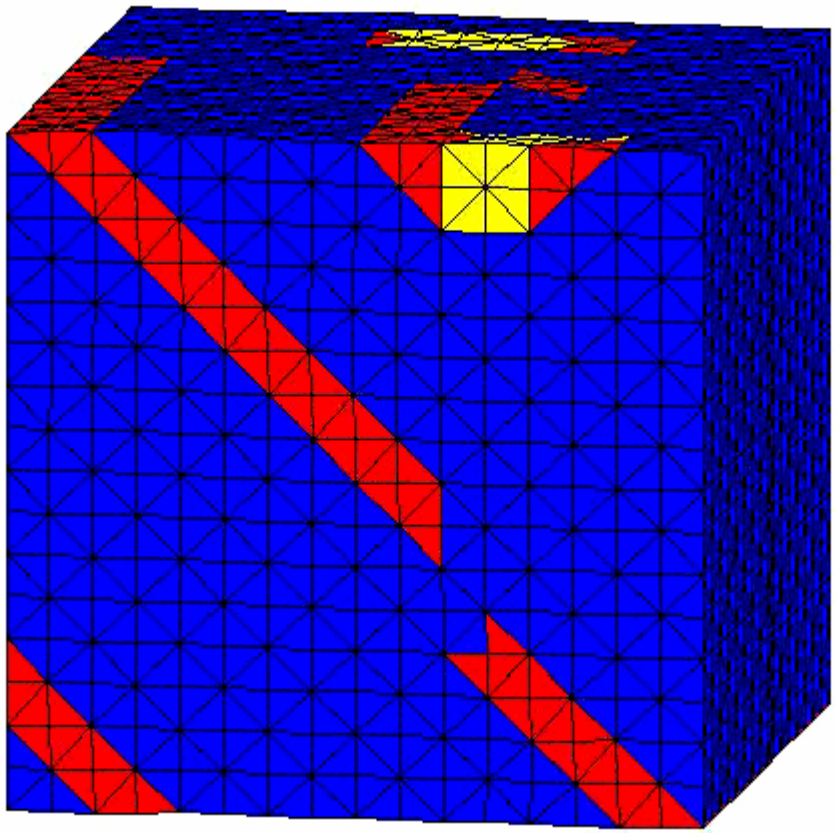
Employ simulated annealing technique:
At each time step j:

- generate random perturbation y* from $y^{(j-1)}$
- if $V(y^*)<V(y^{(j-1)})$: always accept
  otherwise: accept with probability

$$\exp\left(\frac{V(y^{(j-1)}) - V(y^*)}{k}\right)$$

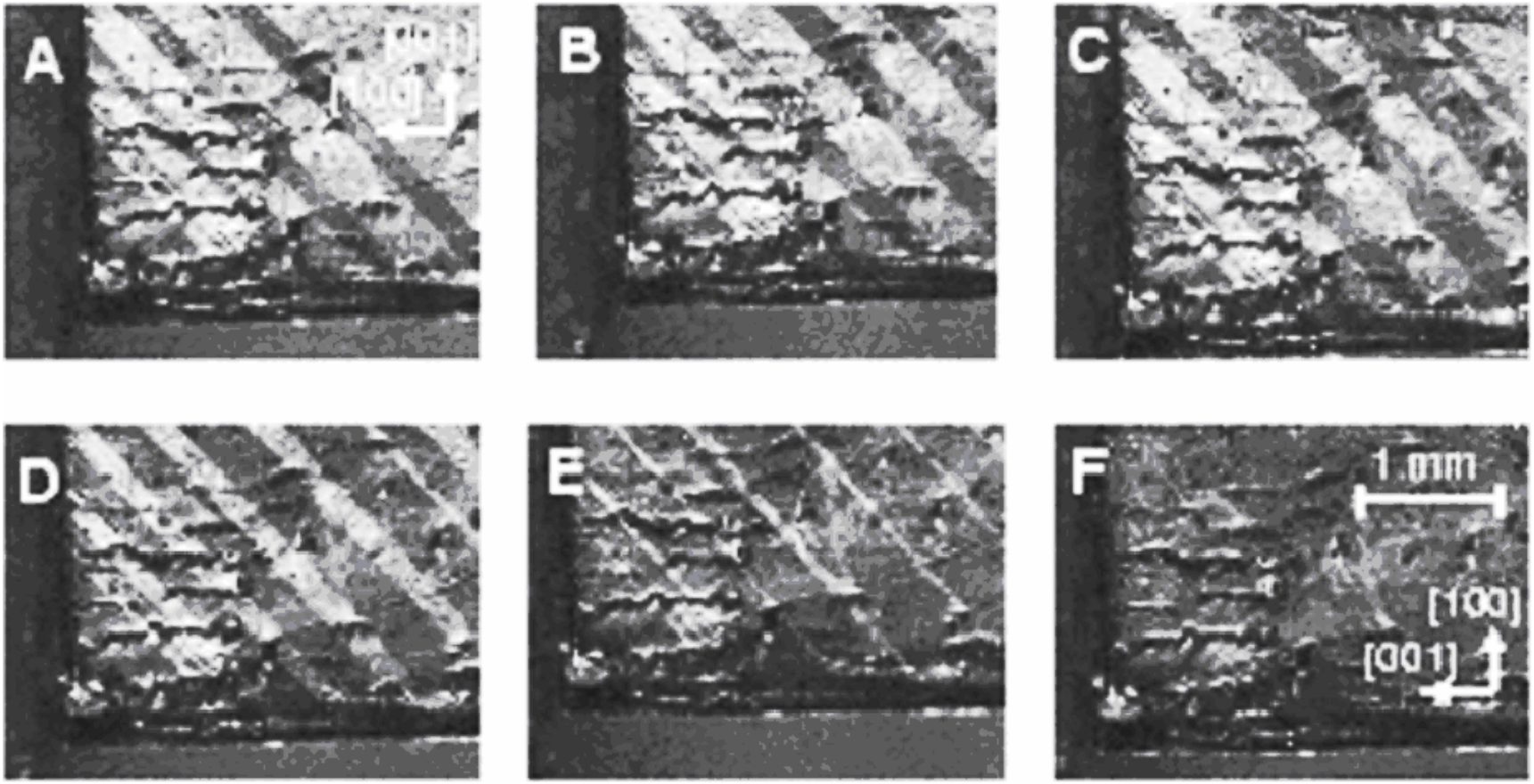
- Repeat this several times
- Local minimization with gradient method

Part III: Experimental and Numerical Results



Laboratory experiment:

Martensite/martensite transformation at 20°C.
Change of microstructure under compression



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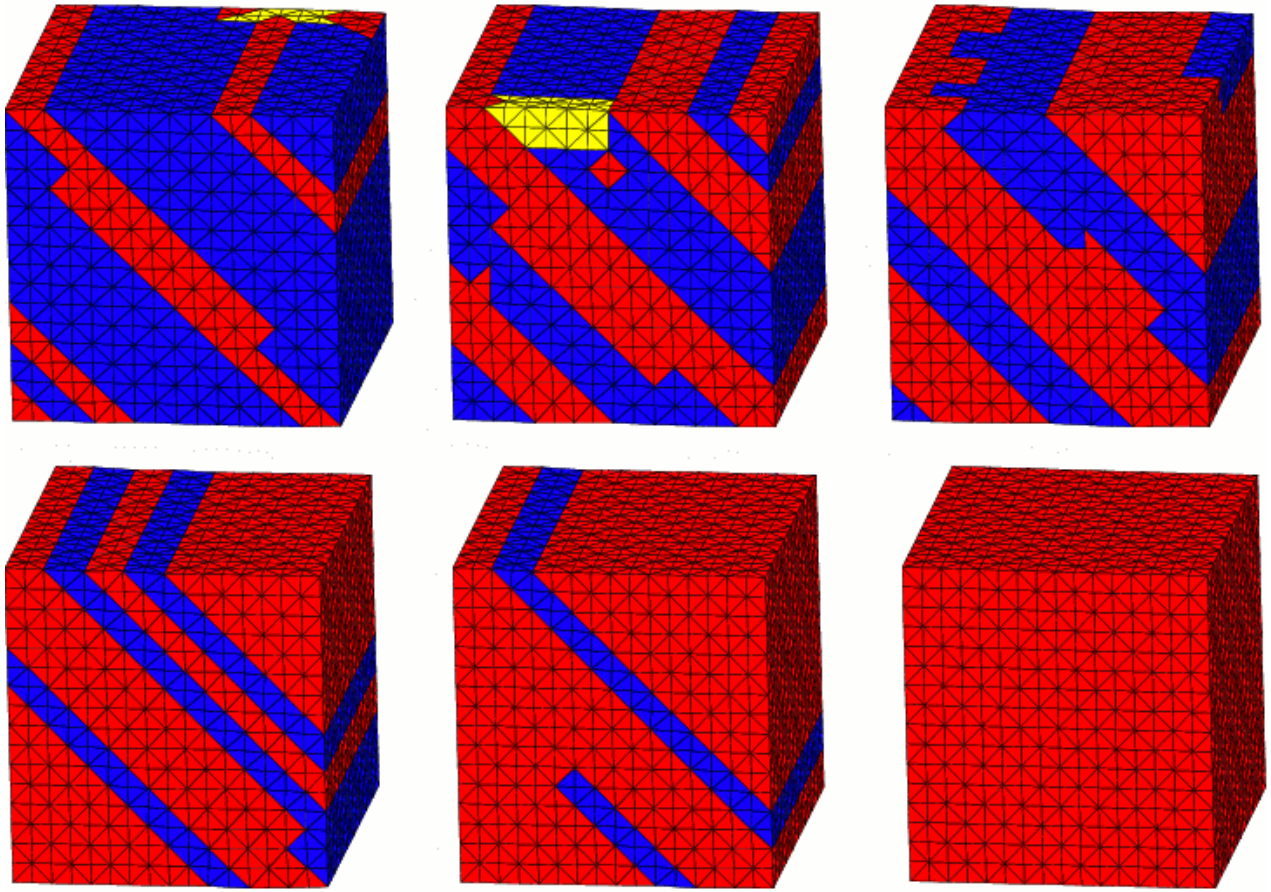
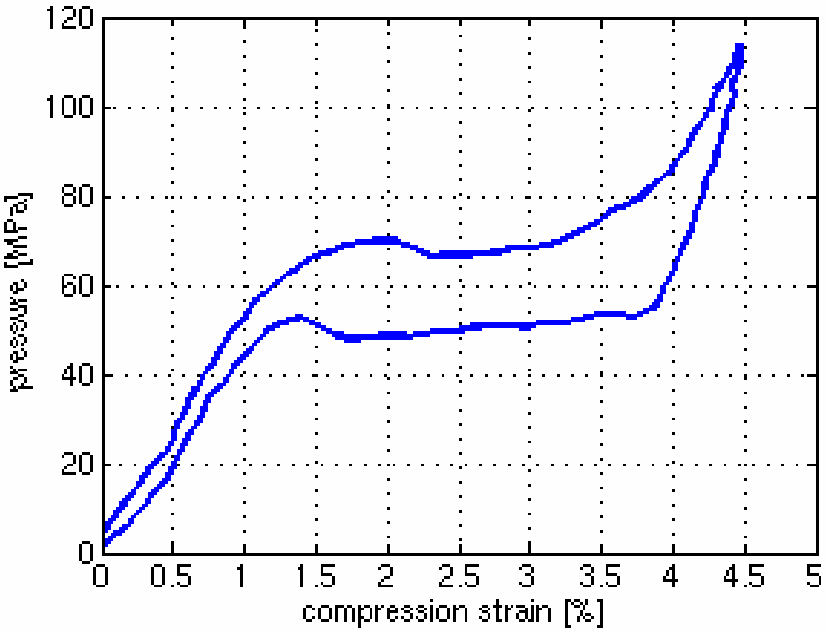
Numerical simulation:

Martensite/martensite transformation at 20°C.
Change of microstructure under compression

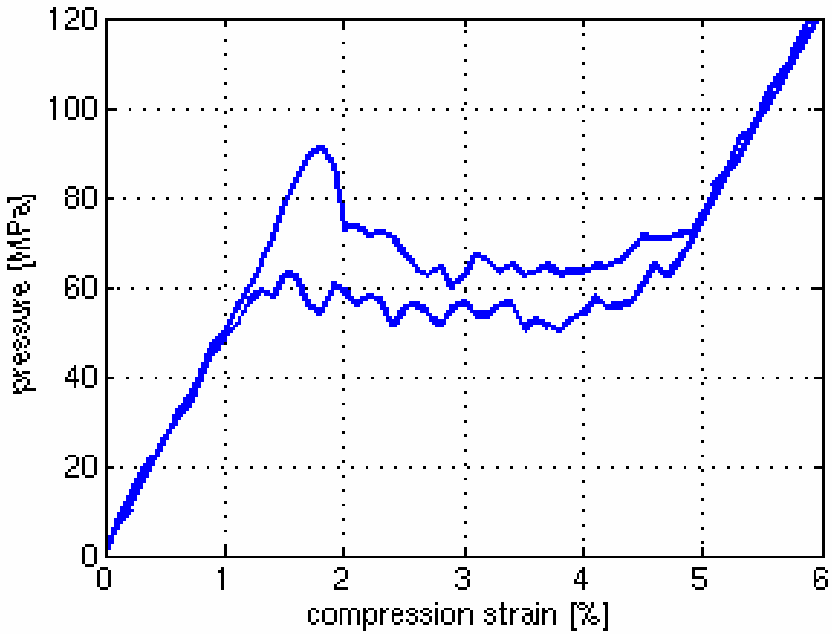


Stress-strain diagram for compression experiment:

Austenite/martensite transformation at 50°C



laboratory experiment



numerical simulation

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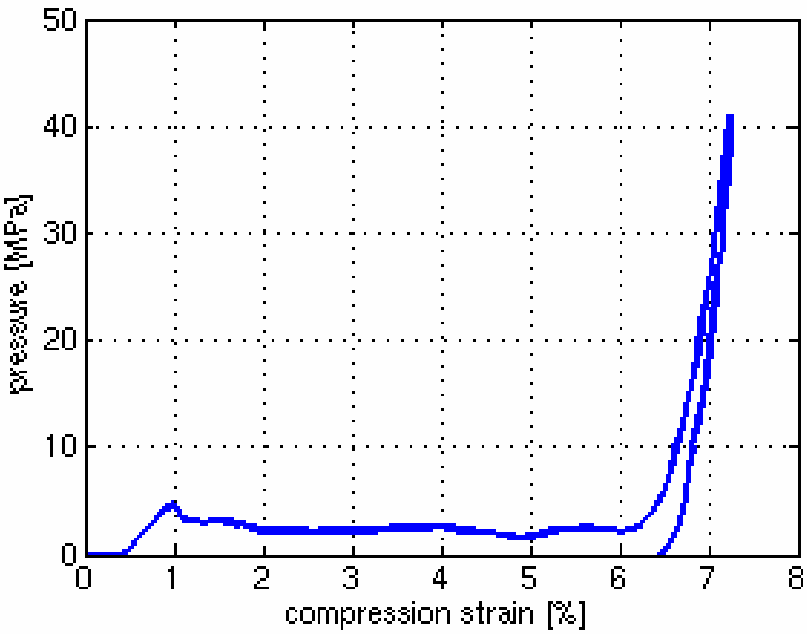
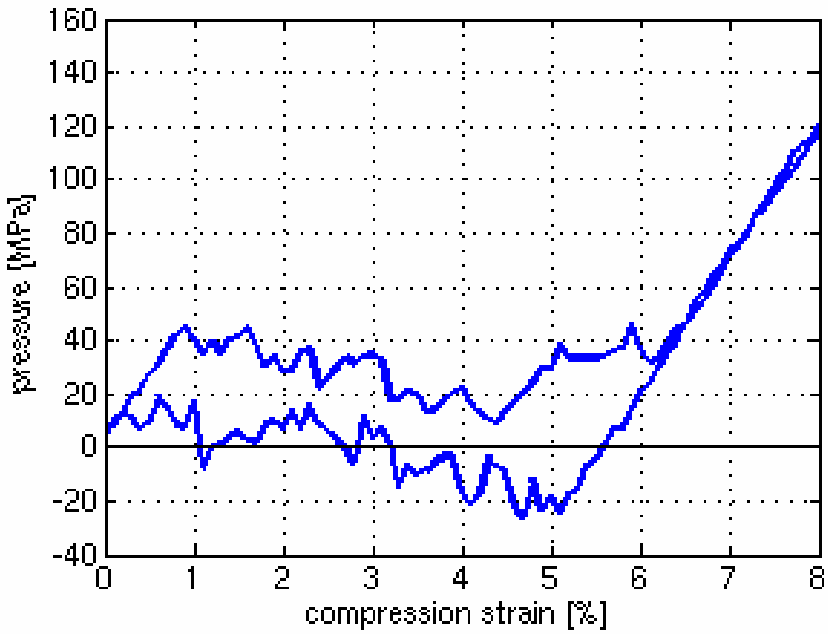
Stress-strain diagram for compression experiment:

Martensite/martensite transformation at 20°C



laboratory experiment

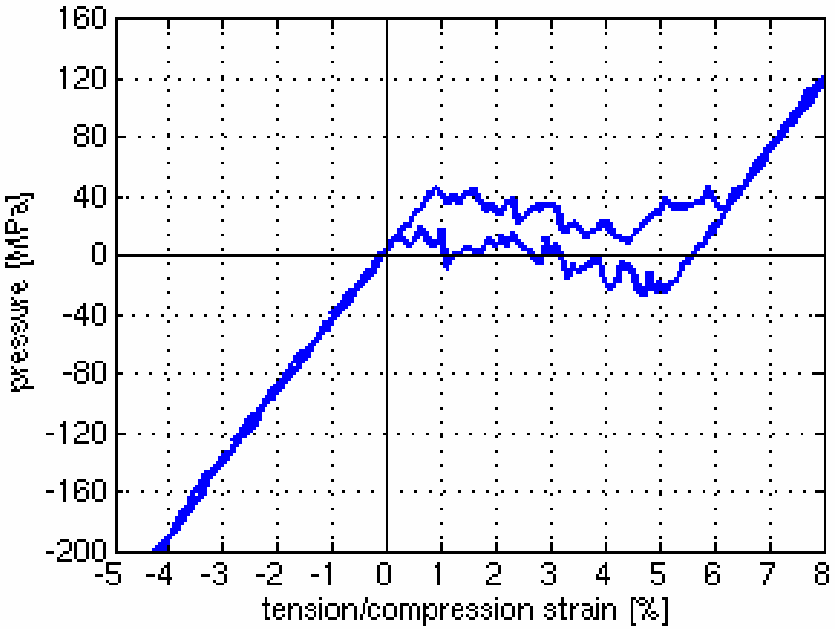


numerical simulation

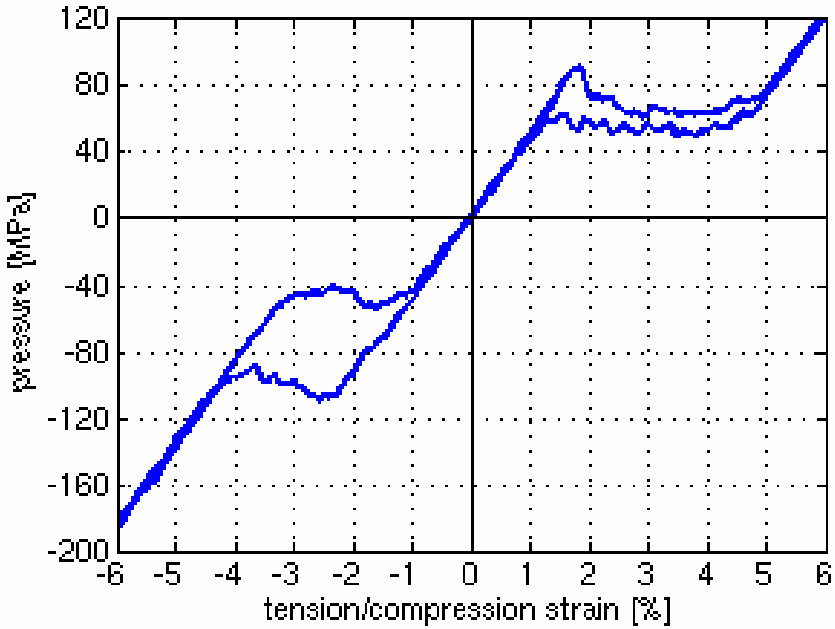
Up to now: compression experiments.
Question: What happens under tension?

- Laboratory experiment:
  Specimen needs to be fixed to loading machine.
  But super-strong and rigid glue etc. not available.
  Tension experiment in laboratory impossible.
- Numerical simulation:
  Tension loading is no problem.
  Model parameters have already been fitted for compression.
  → Use it for tension experiment as well
  → Prediction of SMA behavior under tension!

Numerical simulation of
compression and tension experiment:
Prediction of behavior of our NiMnGa specimen.



M/M transformation
at 20°C



A/M transformation
at 50°C