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

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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
Multi-Scale Modeling

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)
  - Inner expansion technique (A., Griebel 2004)
  - Quasi-continuum method (Tadmor, Ortiz, Phillips 1996)

• **Coupling** of different models within one simulation
  - Heterogeneous Multiscale Method (W. E et. al 2003)

• Analytical Methods:
  - $\Gamma$-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:

\[ W_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad W_1 = \begin{pmatrix} \eta_2 & 0 & 0 \\ 0 & \eta_1 & 0 \\ 0 & 0 & \eta_1 \end{pmatrix} \quad \eta_1 = a_M/a_0 = 1.018 \]
\[ \eta_2 = c_M/a_0 = 0.961 \]
\[ a_0 = 5.839\text{Å} \quad a_M = 5.945\text{Å} \quad c_M = 5.610\text{Å} \]
Modeling: Elastic Energy

• Quadratic form of elastic energy density for each austenite/martensite variant $\alpha$:

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

• Overall elastic energy:

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

$$= \int_{\Omega} \min_{\alpha=0,\ldots,3} (\varphi_\alpha(\nabla y(x)) + \psi_\alpha(\theta)) \, dx$$

• Temperature-dependent offset:

$$\psi_{1,2,3}(\theta) = C(\theta - \theta_{eq}) \quad \text{C=Clausius-Clapeyron slope}$$

$$\psi_{0}(\theta) = 0 \quad \theta_{eq}=\text{equilibrium temperature}$$

• Elastic stress tensor:

$$\sigma_{el} = \frac{\partial}{\partial \nabla y} \varphi(\nabla y, \theta)$$
Modeling of dissipation:

- Observation:
  - 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

\[ \lambda_{\alpha} : \mathbb{R}^{3\times3} \rightarrow \mathbb{R} \]

for each variant \( \alpha=0,1,2,3 \), which fulfill

- \( \lambda_{\alpha} = 1 \) nearby of well \( W_{\alpha} \)
- \( \lambda_{\alpha} = 0 \) far away from well \( W_{\alpha} \)
- smoothly interpolated
Modeling: Dissipation

- Introduce dissipation potential:
  \[ \xi : \mathbb{R}^4 \to \mathbb{R} \quad \xi(z) = \sum_{\alpha=0}^{3} \mathcal{E}_\alpha |z_\alpha| \]

- Dissipation rate:
  \[ \xi \left( \frac{\partial}{\partial t} \lambda(\nabla y) \right) \]
  constants describing the amount of dissipation

- Dissipated energy over time interval \([t_1, t_2]\):
  \[ \xi \left( \text{Var}_{[t_1, t_2]} \lambda(\nabla y) \right) \]
  (Note: total variation is a rate-independent quantity!)

- Associated quasiplastic stress tensor:
  \[ \sigma_{pl} \in \partial \xi \left( \frac{\partial}{\partial t} \lambda(\nabla y) \right) \cdot \lambda'(\nabla y) \]
• Putting it together: \textit{Evolution equation}

\[ \rho \frac{\partial^2 y}{\partial t^2} = \text{div} \left( \sigma_{el}(\nabla y) + \sigma_{pl}(\nabla y, \frac{\partial}{\partial t} \nabla y) \right) \]

\[ \rho = \text{mass density} \]

• Transformation process in SMA experiments here is very slow
  \[ \rightarrow \text{Mass density } \rho \text{ can be neglected.} \]

\[ 0 = \text{div} \left( \sigma_{el}(\nabla y) + \sigma_{pl}(\nabla y, \frac{\partial}{\partial t} \nabla y) \right) \]
Initial conditions:
• Prescribe deformation and velocity at $t=0$

Boundary conditions:
• Time-dependent **Dirichlet** boundary conditions at fixed boundary part $\Gamma_0$:
  $$y(x, t) = y_0(x, t), \quad x \in \Gamma_0 \subset \partial\Omega$$

• Homogeneous **Neumann** boundary conditions at free boundary part $\Gamma_1$:
  $$\nabla y(x, t) \cdot \nu = 0, \quad x \in \Gamma_1 = \partial\Omega \setminus \Gamma_0$$
Part II: Numerical Implementation

Goal: Solve evolution equation numerically.

Discretization in space:
• Decomposition of domain $\Omega$ into tetrahedra
• **Finite Element** method with
  P1 Lagrange ansatz functions:
  • piecewise linear on each tetrahedron
  • continuous on whole domain $\Omega$
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

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

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
  \[ y^{(j-1)} - s^{(j)} \nabla V(y^{(j-1)}), \quad s^{(j)} \in \mathbb{R} \]
- Determination of step size $s^{(j)}$ by **modified Armijo method:**
  \[
  s^{(j)} = s^{(j-1)} \max\{2^i : i \in \mathbb{Z} \text{ and } \forall k \in [\min(0, i), i] \cap \mathbb{Z} : \\
  V\left( y^{(j-1)} - 2^k s^{(j-1)} \nabla V(y^{(j-1)}) \right) \leq V(y^{(j-1)}) - \beta 2^k s^{(j-1)} \| \nabla V(y^{(j-1)}) \|^2 \}
  \]
- 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
Numerical simulation:
Martensite/martensite transformation at 20°C.
Change of microstructure under compression
Experimental and Numerical Results

Stress-strain diagram for compression experiment:

Austenite/martensite transformation at 50°C
Experimental and Numerical Results

Stress-strain diagram for compression experiment:

Martensite/martensite transformation at 20°C

![Stress-strain diagram](image)

- laboratory experiment
- numerical simulation
Experimental and Numerical Results

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