Modeling Phase Transitions in Shape Memory Alloys

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Solution Methods for Large-Scale Nonlinear Problems
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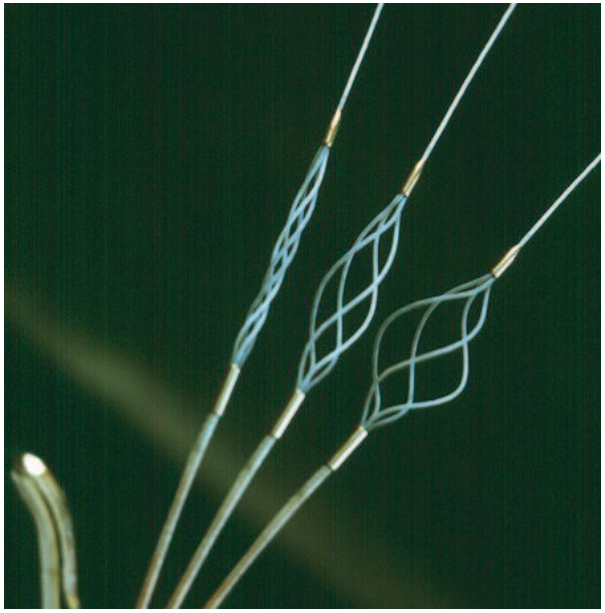
"Smart" Materials and Potential Applications

Active materials exhibit a dramatic, controllable phase transformation

Shape Memory Alloys (SMA):

- thermal → mechanical work
- First discovered in 1932 by A. Ölander
- Came to forefront of materials research in 1960s [W.J. Buehler]
- Potential for: vibration damping, nanomachinery

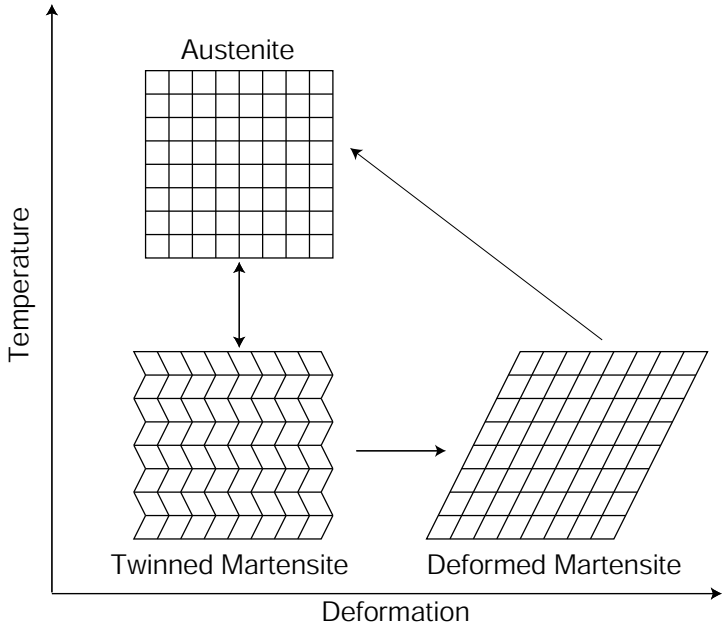


SMA Arterial Stent
(from smet.tomsk.ru)

Other active materials with similar phase transformation behavior include Ferromagnets, Piezoelectrics.

First-Order Martensitic Phase Transformation

Materials change elasticity, crystal structure according to temperature and stress:



Shape Memory Effect
(adapted from J. Ryhänen)

Austenite:

- High Symmetry (cubic)
- Single Structure
- Stiff ($\sim$ Titanium)

Martensite:

- Low Symmetry (tetragonal)
- Multiple Structures
- Ductile ($\sim$ Soft Pewter)
- Deformations Move Twinning Planes

General Thermodynamic Model

Continuum thermodynamic description given by the nonlinear system

$$\begin{aligned}
&\text{(velocity)} && \dot{u} = v, \\
&\text{(viscoelastic)} && \rho_0 \dot{v} = \rho_0 \partial^2_{x\gamma} \Psi + \alpha\, \partial^2_{xx} v + \rho_0 b, \\
&\text{(energy)} && \rho_0 c_p \dot{\theta} = \rho_0\, \theta\, \partial^2_{\gamma\theta} \Psi\, \dot{\gamma} + \alpha\, (\dot{\gamma})^2 + \kappa\, \partial_x \left(\gamma\, \partial_x \theta\right) + \rho_0 r,
\end{aligned}$$

where $(x, t) \in [0, L] \times I\!R^+$.

We subject the wire to

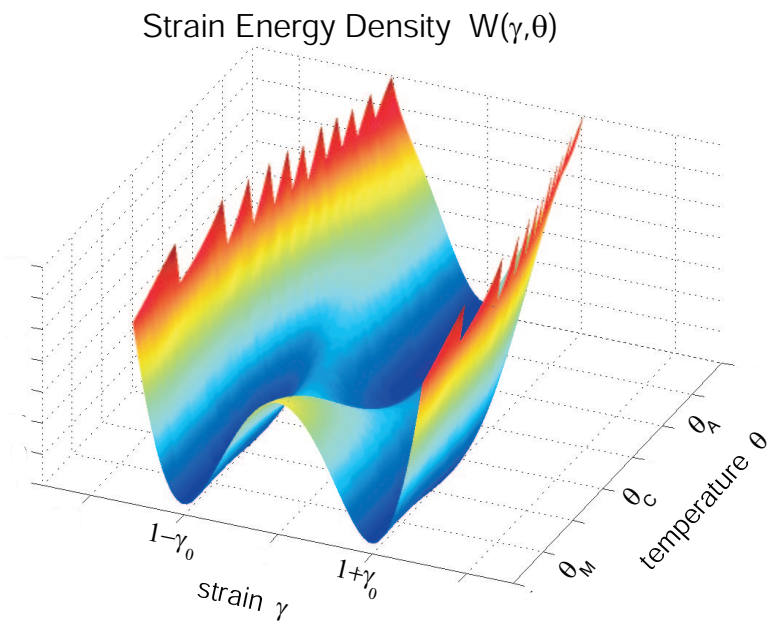
- Given initial conditions $\{u_0, v_0, \theta_0\}$,
- Boundary conditions corresponding to fixed left end of wire, free right end of wire in both space and temperature.

The Helmholtz Free Energy

Material physics described through an expanded form of the Landau-Devonshire potential:

$$\Psi(\gamma,\theta) = \mathcal{W}(\gamma,\theta) + c_p\theta(1-\ln\theta) + D\theta + E,$$

$$\mathcal{W}(\gamma,\theta) = \mathcal{W}_M(\gamma)C_M(\theta) + \mathcal{W}_C(\gamma)C_C(\theta) + \mathcal{W}_A(\gamma)C_A(\theta)$$



$\mathcal{W}_*(\gamma)$ – isothermal elastic profiles
$C_*(\theta)$ – smoothly connect in θ

Strain energy density $\mathcal{W}(\gamma,\theta)$ provides material phase transformation and satisfies all measurable material constants for stable states.

Treatment of the Mathematical Model

Weak solution u, v, θ to nonlinear system

$$\begin{aligned}
\dot{u} &= v, \\
\rho_0 \dot{v} &= \rho_0 \partial^2_{x\gamma} \Psi + \alpha\, \partial^2_{xx} v + \rho_0 b, \\
\rho_0 c_p \dot{\theta} &= \rho_0\, \theta\, \partial^2_{\gamma\theta} \Psi\, \dot{\gamma} + \alpha\, (\dot{\gamma})^2 + \kappa\, \partial_x\, (\gamma\, \partial_x \theta) + \rho_0 r
\end{aligned}$$

Requires:

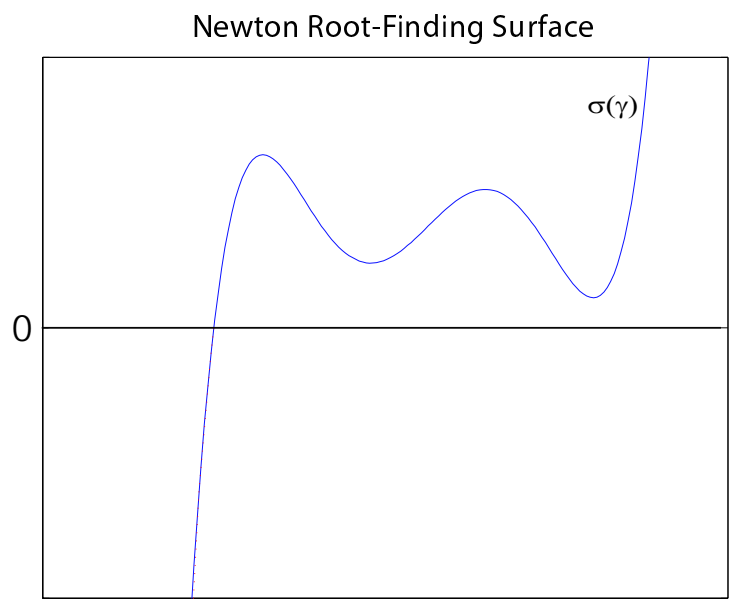
- Space-discretization – piecewise-affine finite elements (limited regularity of expected weak solutions)
- Time-discretization – continuous-time Galerkin method (discrete Lyapunov function, uniform treatment of space/time)
- Nonconvex optimization – continuation method utilizing viscosity-regularized solutions and Newton's method
- Linear systems – sparse, non-restarted GMRES using ILU precond.

Nonlinear Instabilities

Desire "small" viscosity solutions: physical experiments observe little or no viscous effects [Seelecke, Heintze, Bergman 2003]

However, small α induce:

- Inflection points at moment of phase transition
- Numerical instability in Newton method iterates.



Unsuccessful 'Black Box' Attempts

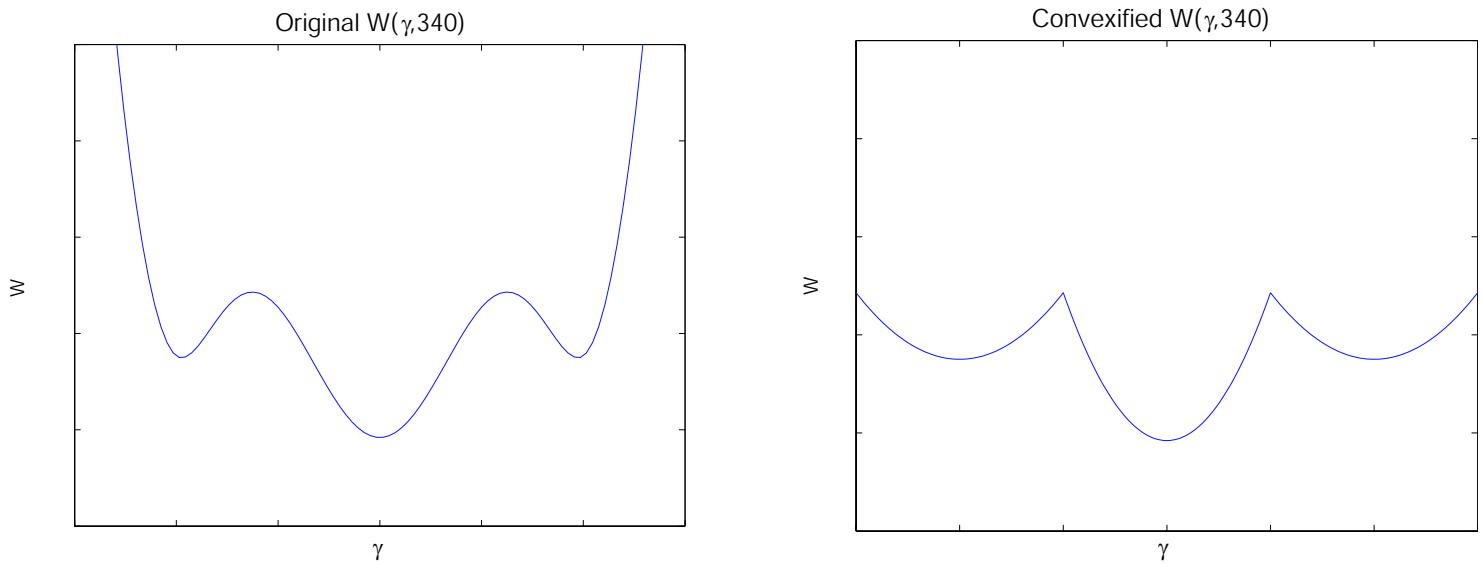
- Damped Newton Algorithm:
  - Combines Newton with a standard linesearch algorithm
  - Stagnates iterates at the inflection point (phase transition)
- Tunneling Newton Algorithm [Levy, Gomez] and Terminal Repeller [Cetin, Barhen, Burdick]:
  - Replaces root-finding problem $f(x) = 0$ with e.g.

$$\hat{f}(x) = \frac{f(x) - f(x_s)}{\|x - x_s\|^{\alpha}} = 0$$

  - Unreliable on large-scale problems (> 10 opt. variables)
  - Highly dependent on *tuning parameters* to provide reasonable pole locations, strengths and restarting values

Unsuccessful Attempts (Continued)

- Newton with Physically-Intuitive Restarts:
  - At transition, restart Newton with iterate in newly stable phase
  - Difficult to algorithmically account for full nonlinear effects
- Piecewise Convexification of Strain Energy $\mathcal{W}(\gamma, \theta)$:
  - Use piecewise convex projection of $\mathcal{W}$ to get past transition



  - Deviates too far from physics to remain relevant

Variable Viscosity Newton Method

Resolve instabilities through changing viscosity level:

1. Keep viscosity low/zero until phase transition
2. Increase viscosity to remove instability
   i.e. add weighted Laplacian to smooth out nonlinearity
3. Progressively decrease coefficient α to "pull" perturbed solution over energy barrier toward zero-viscosity solution

Similar to other methods for nonlinear problems:

- Method of Vanishing Viscosity [Hopf 1950; Lax 1954] for scalar hyperbolic equations
- Traditional regularization methods used for inverse problems

Variable Viscosity Newton Method (Continued)

Benefits over other solution methods:

- Considerably smaller final viscosity than prescribed by theory
- Inflated viscosity necessary only for short period of time
- Viscous effects on overall system are measurable
- Resulting algorithm much faster than other global methods (Simulated Annealing, Genetic Algorithms)

Performance figures:

- During "normal" time steps, takes $\sim$3 Newton steps and $\sim$7 Krylov iterations per Newton step
- During phase transitions, same figures as above for each viscosity level, and $\sim$5 viscosity levels per time step

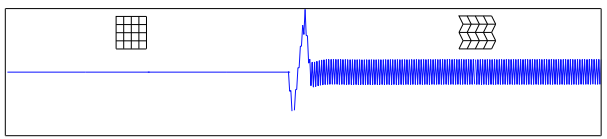
Computations and Visualization

1-D deformation constitutes elongation/contraction

Displacement plotted for clarity:

positive = elongation

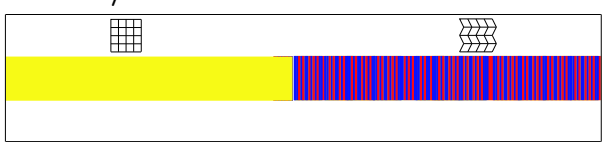
negative = contraction



Phase plots:

Yellow = austenite

Red/Blue = martensite$^{\pm}$

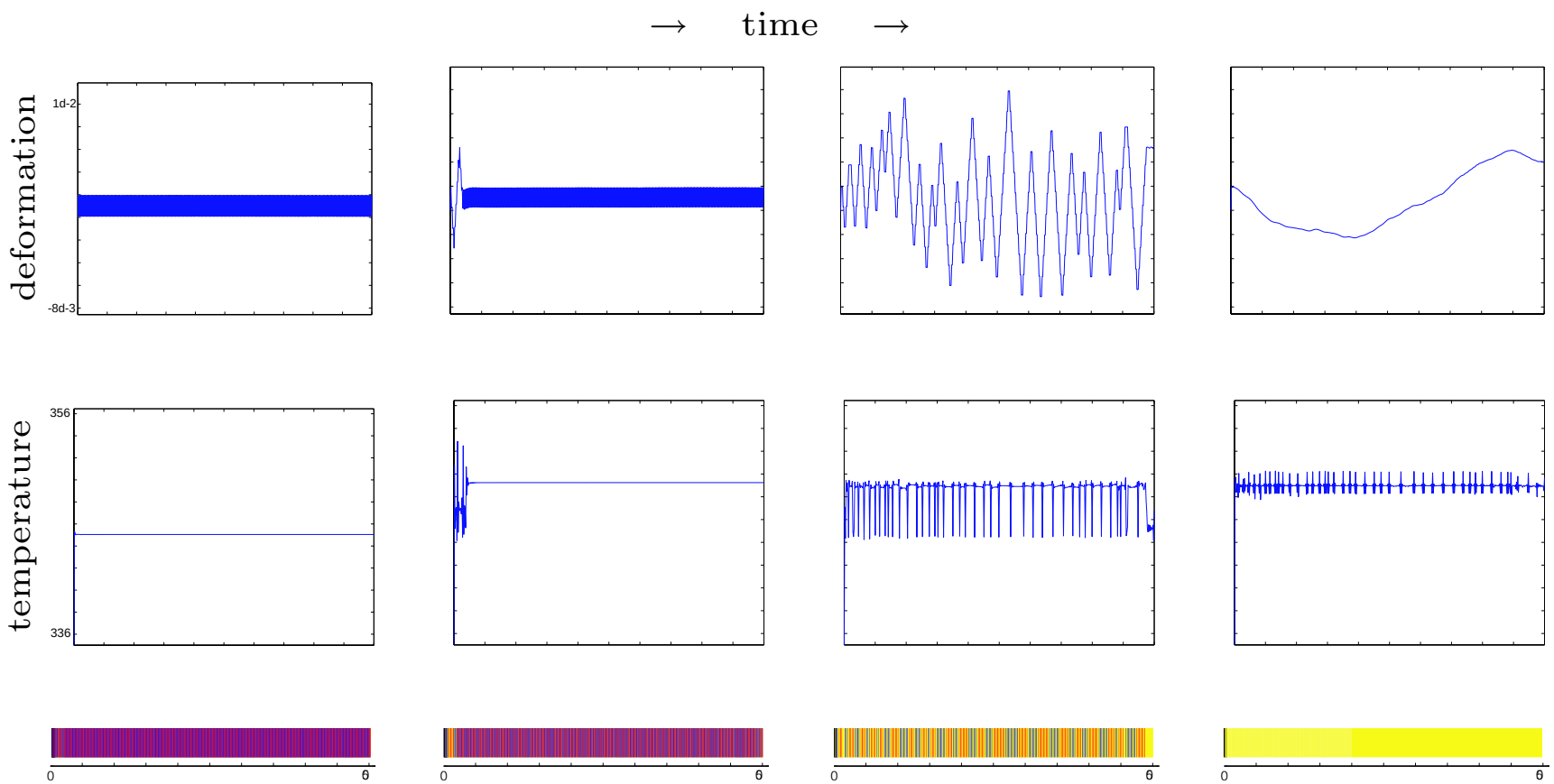


Constant	Value
Δx	10 μm
Δt	1 μs
ρ_0	$6.45 * 10^3$ kg m^{-3}
κ	10 W (m K)$^{-1}$
c_p	322 J (kg K)$^{-1}$
E_a	$7.5 * 10^{10}$ Pa
E_m	$2.8 * 10^{10}$ Pa
θ_A	350 K
θ_C	335 K
θ_M	320 K

NiTi simulation constants

Results – Martensite to Austenite Transformation

Heat supply $r(x,t)$ positive and constant.



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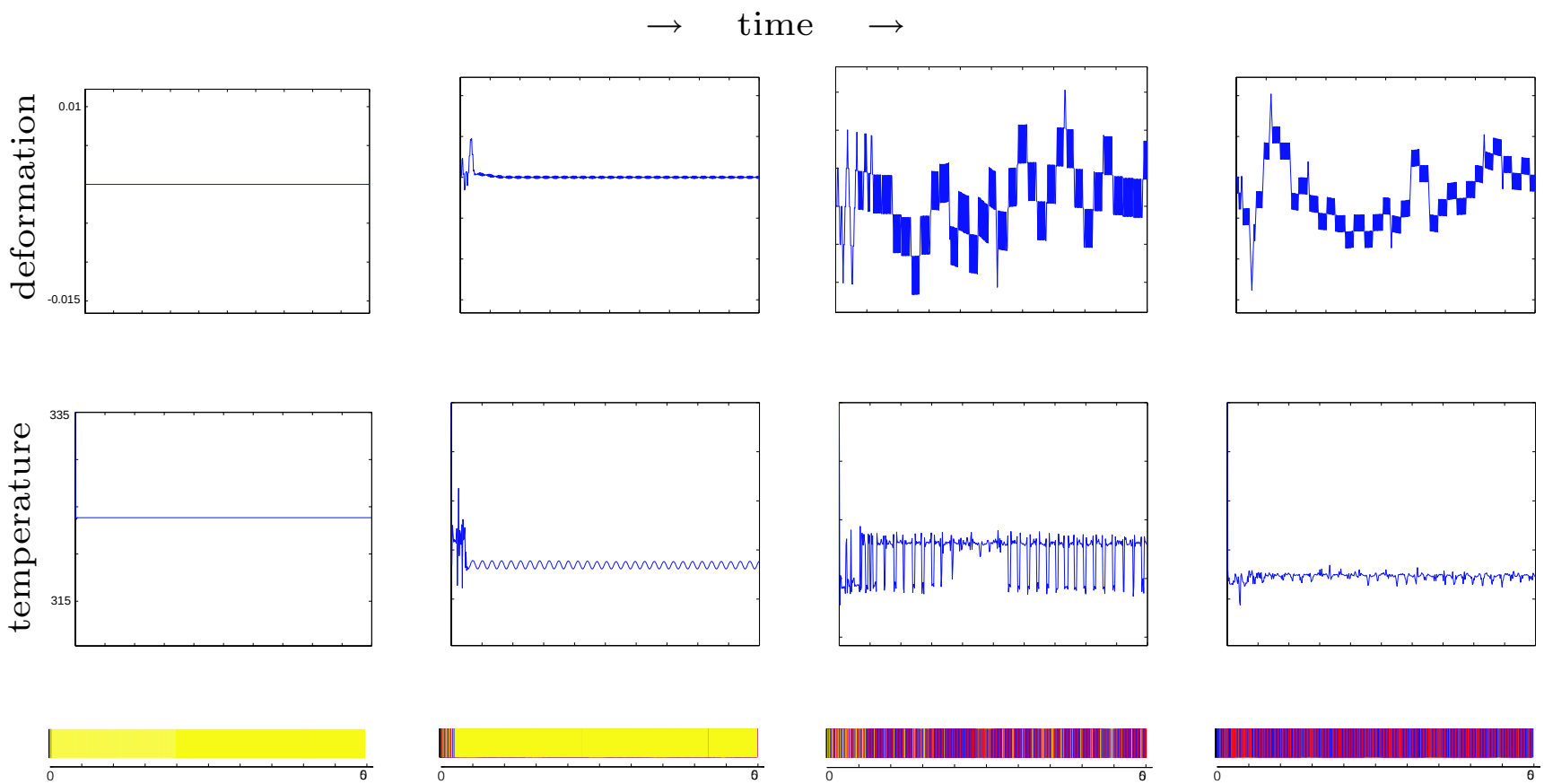
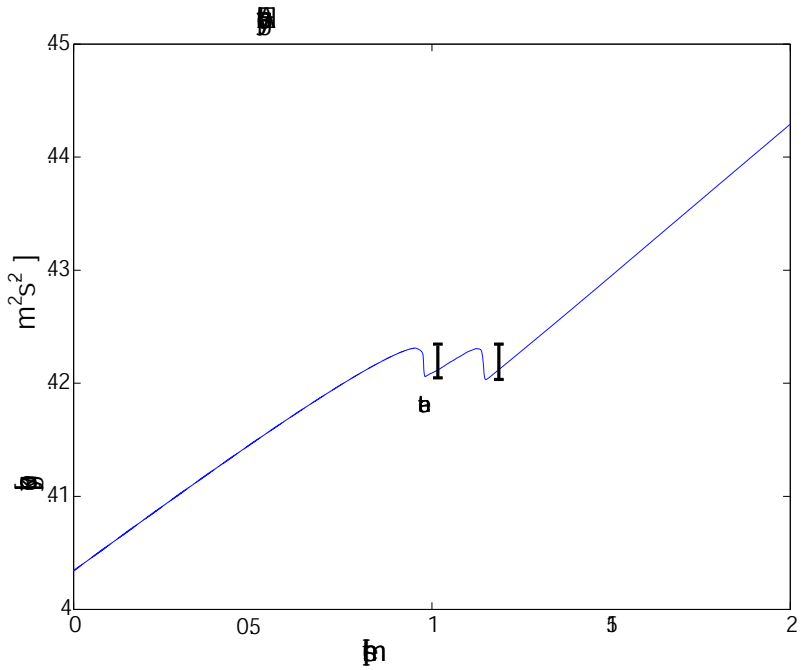
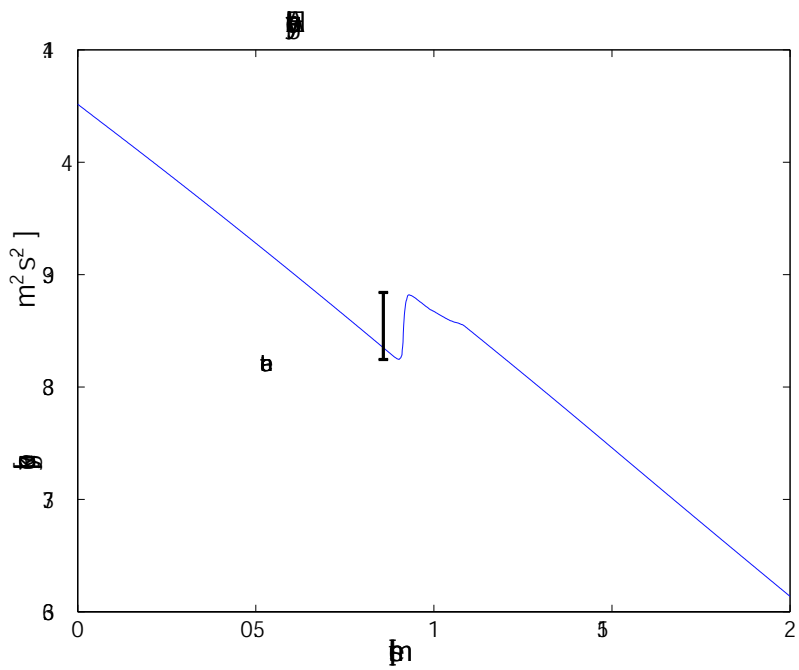


Latent Heat

Nonlinear latent heat effects are measured by enthalpy jumps. Model successfully predicts these for thermally-induced transformations:



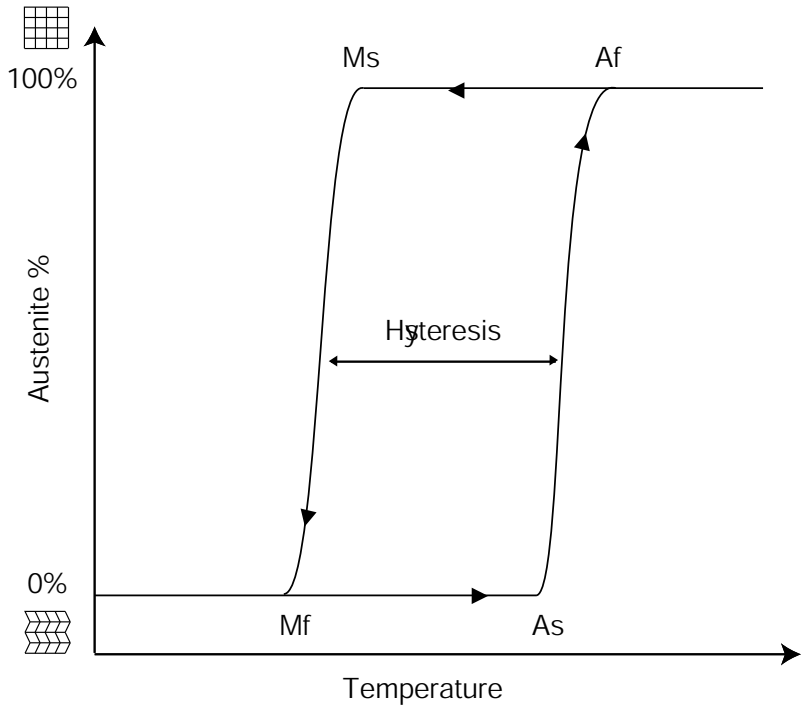
Martensite → Austenite Enthalpy



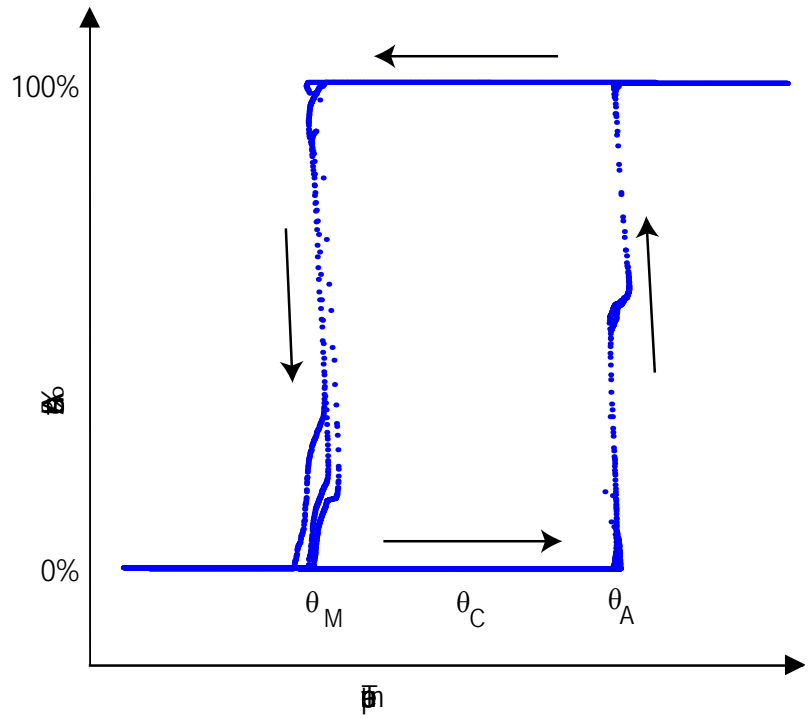
Austenite → Martensite Enthalpy

Hysteresis Test

Model predicts nonlinear hysteretic effects, which measure possible thermal → mechanical work:



Ideal Hysteresis Loop



Computed Hysteresis Loop

Benefits and Limitations of This Approach

(+) Clean, predictive approach to thermodynamic modeling of phase transitions

(+) Successfully describes both phases of SMA, crystalline phase transformation, material properties, large temperature range

(±) All material physics included in the Helmholtz free energy

(−) Does not account for polycrystalline structure and material defects of production alloys

(−) One-space dimension loses some physics of full material transformation

Directions for Future Research

- Improve the nonlinear, nonconvex solver to provide scalability to higher dimensions
- Further validation and tuning of free energy with physical experiments
- Extend modeling system to thin films (2-D) and solids (3-D)
- Examine approaches based on a stochastic description of free energy (polycrystalline materials, defects)

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