Modeling and Simulation of Microstructured Magnetic Shape Memory Materials

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MAGNETIC SHAPE MEMORY
A DFG PRIORITY PROGRAMME
Overview

1. Introduction

2. Modeling Equilibrium Configurations
   - Micromagnetic–Elastic Model
   - Rigid Particles and Linear Elasticity
   - Discretization and Energy Descent
   - Results

3. Rate-Independent Dynamics
   - 1D Example
   - Modeling Twin Boundary Motion
   - Twin Boundary Motion & Hysteresis
Introduction

Polycrystals and Composites

Microstructures in MSM Materials: Polycrystals and Composites
Microstructures in MSM Materials: Polycrystals and Composites

**Polycrystals**
Incompatibilities at grain boundaries lead to smaller deformations
Polycrystals and Composites

Microstructures in MSM Materials: Polycrystals and Composites

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Microstructures in MSM Materials: Polycrystals and Composites

**Polycrystals**
Incompatibilities at grain boundaries lead to smaller deformations

**Composites**
Polymer matrix accommodates deformation of small particles

[Gutfleisch et al.]
Microstructures in MSM Materials: Polycrystals and Composites

**Polycrystals**
Incompatibilities at grain boundaries lead to smaller deformations

**Composites**
Polymer matrix accommodates deformation of small particles [Gutfleisch et al.]
**Polycrystals**

- **Blue:** Magnetic Shape–Memory Material
- **Yellow–Red:** Background Matrix

Shading encodes elastic energy density (dark for high energy)
Grid shows crystal lattice orientation and deformation

**Composites**
2-Dimensional Model of the Phase Transformation

Martensitic Variants

\[
\begin{align*}
\bar{\varepsilon}_1 &= \left( \varepsilon_0 0 0 - \varepsilon_0 \right) \\
\bar{\varepsilon}_2 &= \left( 0 0 - \varepsilon_0 \varepsilon_0 \right)
\end{align*}
\]
Modeling Equilibrium Configurations ➥ Micromagnetic–Elastic Model

2-Dimensional Model of the Phase Transformation

Martensitic Variants

Linearized Elastic Transformation Strain

\[ \bar{\varepsilon}_1 = \left( \begin{array}{cc} \varepsilon_0 & 0 \\ 0 & -\varepsilon_0 \end{array} \right) \]

\[ \bar{\varepsilon}_2 = \left( \begin{array}{cc} -\varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{array} \right) \]
### 2-Dimensional Model of the Phase Transformation

#### Martensitic Variants

#### Linearized Elastic Transformation Strain

\[
\bar{\varepsilon}_1 = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & -\varepsilon_0 \end{pmatrix} \quad \bar{\varepsilon}_2 = \begin{pmatrix} -\varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{pmatrix}
\]

#### Anisotropy for the Magnetization \( m \)

\[
\gamma_1(m) = m_1^2 \quad \gamma_2(m) = m_2^2
\]
\[ E[v, m, p] = E_{\text{elast}} + E_{\text{polymer}} + E_{\text{elast}} + E_{\text{MSM}} + E_{\text{ext}} + E_{\text{demag}} + E_{\text{anis}} + E_{\text{exch}} \]

\[ = \int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) + \int_{\omega} W_{\text{MSM}}((\nabla v)Q, p) - \int_{\nu(\omega)} H_{\text{ext}} \cdot m + \int_{\mathbb{R}^d} \frac{1}{2} |H_d|^2 + \int_{\nu(\omega)} \gamma_p((RQ)^T m) + \int_{\nu(\omega)} \frac{1}{2} d^2 |\nabla m|^2 \]

\(\Omega \subset \mathbb{R}^d\) area occupied by composite
\(\omega \subset \Omega\) area occupied by particles
\(\omega = \Omega\) for polycrystals


\[ E[v, m, p] = E_{\text{polymer}}^{\text{elast}} + E_{\text{MSM}} + E_{\text{ext}} + E_{\text{demag}} + E_{\text{anis}} + E_{\text{exch}} + \int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) \]

- \( \Omega \subset \mathbb{R}^d \) area occupied by composite
- \( \omega \subset \Omega \) area occupied by particles
- \( \omega = \Omega \) for polycrystals

**Matrix Elasticity**
(only in composites)

\[ W_{\text{polymer}} \] stored energy density of polymer bulk

\[ v : \Omega \rightarrow \mathbb{R}^d \] deformation
Modeling Equilibrium Configurations ➞ Micromagnetic–Elastic Model

Full Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{elast}}^{\text{polymer}} = \int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) + \int_{\omega} W_{\text{MSM}}((\nabla v)Q, p) + E_{\text{ext}} - \int_{v(\omega)} H_{\text{ext}} \cdot m + \int_{\mathbb{R}^d} \frac{1}{2} |H_d|^2 + \int_{v(\omega)} \gamma_p((RQ)^T m) + \int_{v(\omega)} \frac{1}{2} d^2 |\nabla m|^2 + E_{\text{demag}} + E_{\text{anis}} + E_{\text{exch}} \]

\( \Omega \subset \mathbb{R}^d \) area occupied by composite
\( \omega \subset \Omega \) area occupied by particles
\( \omega = \Omega \) for polycrystals

Particle / Grain Elasticity

\( W_{\text{MSM}} \) stored energy density of particles / grains, i.e. quadratic distance to eigenstrain with respect to crystal lattice orientation

\( p : \omega \to \{1, \ldots, d\} \) phase parameter in particles / grains
\( Q : \omega \to \text{SO}(d) \) lattice orientation in particles / grains
\( v : \Omega \to \mathbb{R}^d \) deformation
Full Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{elast}}^\text{polymer} + E_{\text{elast}}^\text{MSM} + E_{\text{ext}} + E_{\text{demag}} + E_{\text{anis}} + E_{\text{exch}} = \int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) + \int_{\omega} W_{\text{MSM}}((\nabla v)Q, p) - \int_{v(\omega)} H_{\text{ext}} \cdot m + \int_{\mathbb{R}^d} \frac{1}{2} |H_d|^2 + \int_{v(\omega)} \gamma_p((RQ)^T m) + \int_{v(\omega)} \frac{1}{2} d^2 |\nabla m|^2 \]

\( \Omega \subset \mathbb{R}^d \) area occupied by composite
\( \omega \subset \Omega \) area occupied by particles
\( \omega = \Omega \) for polycrystals

Interaction with External Field

\( m : v(\omega) \to \mathbb{R}^d \) magnetization
\( H_{\text{ext}} \in \mathbb{R}^d \) external magnetic field
Modeling Equilibrium Configurations ➞ Micromagnetic–Elastic Model

Full Model for Micromagnetism and Elasticity

\[
E[v, m, p] = E_{\text{polymer}}^{\text{elast}} + E_{\text{MSM}} + E_{\text{ext}} + E_{\text{demag}} + E_{\text{anis}} + E_{\text{exch}} = \\
\int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) + \int_{\omega} W_{\text{MSM}}((\nabla v)Q, p) - \int_{\nabla v(\omega)} H_{\text{ext}} \cdot m + \int_{\mathbb{R}^d} \frac{1}{2} |H_d|^2 + \int_{\nabla v(\omega)} \gamma_p((RQ)^T m) + \int_{\nabla v(\omega)} \frac{1}{2} d^2 |\nabla m|^2
\]

\( \Omega \subset \mathbb{R}^d \) area occupied by composite
\( \omega \subset \Omega \) area occupied by particles
\( \omega = \Omega \) for polycrystals

Demagnetization

\( m : \ n(\omega) \rightarrow \mathbb{R}^d \) magnetization
\( H_d : \ \mathbb{R}^d \rightarrow \mathbb{R}^d \) demagnetization field

\[ H_d = \nabla \psi \]
\[ \Delta \psi = \text{div} \ m \] distributionally
Modeling Equilibrium Configurations

Micromagnetic–Elastic Model

Full Model for Micromagnetism and Elasticity

\[ E[v, m, p] = \]

\[ E_{\text{polymer}}^{\text{elast}} + E_{\text{MSM}}^{\text{elast}} + E_{\text{ext}} + E_{\text{demag}} + E_{\text{anis}} + E_{\text{exch}} \]

\[ = \int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) \]

\[ + \int_{\omega} W_{\text{MSM}}((\nabla v)Q, p) \]

\[ - \int_{\nu(\omega)} H_{\text{ext}} \cdot m \]

\[ + \int_{\mathbb{R}^d} \frac{1}{2} |H_d|^2 \]

\[ + \int_{\nu(\omega)} \frac{1}{2} d^2 |\nabla m|^2 \]

\[ \Omega \subset \mathbb{R}^d \quad \text{area occupied by composite} \]

\[ \omega \subset \Omega \quad \text{area occupied by particles} \]

\[ \omega = \Omega \quad \text{for polycrystals} \]

Anisotropy

\[ m : \nu(\omega) \rightarrow \mathbb{R}^d \quad \text{magnetization} \]

\[ p : \omega \rightarrow \{1, \ldots d\} \quad \text{phase parameter in particles / grains} \]

\[ \gamma_p : \mathbb{R}^d \rightarrow \mathbb{R} \quad \text{anisotropy in phase } p \]

\[ R \in SO(d) \quad \text{rotational part of deformation } \nabla v = RU \]

\[ Q : \omega \rightarrow SO(d) \quad \text{lattice orientation in particles / grains} \]
Modeling Equilibrium Configurations ➔ Micromagnetic–Elastic Model

Full Model for Micromagnetism and Elasticity

\[ E[v, m, p] = \begin{align*}
E_{\text{polymer}}^{\text{elast}} & + E_{\text{MSM}}^{\text{elast}} \\
+ & E_{\text{ext}} \\
+ & E_{\text{demag}} \\
+ & E_{\text{anis}} \\
+ & E_{\text{exch}} \\
= & \int_{\Omega \setminus \omega} W_{\text{polymer}}(\nabla v) \\
+ & \int_{\omega} W_{\text{MSM}}((\nabla v)Q, p) \\
- & \int_{v(\omega)} H_{\text{ext}} \cdot m \\
+ & \int_{\mathbb{R}^d} \frac{1}{2} |H_d|^2 \\
+ & \int_{v(\omega)} \gamma_p ((RQ)^T m) \\
+ & \int_{v(\omega)} \frac{1}{2} d^2 |\nabla m|^2
\end{align*} \]

\( \Omega \subset \mathbb{R}^d \) area occupied by composite
\( \omega \subset \Omega \) area occupied by particles
\( \omega = \Omega \) for polycrystals

Magnetic Exchange
\( m : v(\omega) \rightarrow \mathbb{R}^d \) magnetization
- Particles are small and hard
  \( \leadsto \) \textbf{particle deformations are affine}

- Particles are single crystals
  \( \leadsto \) \textbf{lattice orientation} \( Q \) \textbf{constant}
    \textbf{on each particle / grain}

- Particles / grains are single-domain
  \( \leadsto \) \textbf{phase} \( p \) \textbf{and magnetization} \( m \) \textbf{constant}
    \textbf{on particles / grains}
  \( \leadsto E_{\text{exch}} = 0 \)

- Deformations are (relatively) small
  \( \leadsto \) \textbf{linearized elasticity}
Large numbers of small particles or grains: Fully resolved simulation not feasible

Homogenization: Study periodic configurations

Consider unit square with some particles or grains, periodic boundary conditions for magnetic field, affine–periodic for deformation
Keep in mind: Computational cell is part of periodic configuration
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Minimize over internal variables

- particle deformation
- particle / grain magnetization
- particle / grain phase
Minimize over internal variables

- particle deformation 6
- particle / grain magnetization 1
- particle / grain phase 1

8 degrees of freedom per particle / grain
Minimize over internal variables

- particle deformation 6
- particle / grain magnetization 1
- particle / grain phase 1

8 degrees of freedom per particle / grain

For a given configuration, the energy now is a function of

- the external magnetic field and
- the macroscopic deformation.
Minimize over internal variables

- particle deformation 6
- particle / grain magnetization 1
- particle / grain phase 1

8 degrees of freedom per particle / grain

For a given configuration, the energy now is a function of

- the external magnetic field and
- the macroscopic deformation.

Energy minimization: **Gradient descent**

- approximate gradient by finite differences
- combinatorial exploration of phase parameters
Energy evaluation: **Boundary Element Method**

**Elasticity in Polymer Matrix**

- Affine-periodic cell boundary
- Dirichlet particle boundary
Energy evaluation: **Boundary Element Method**

**Elasticity in Polymer Matrix**
- Affine-periodic cell boundary
- Dirichlet particle boundary

**Demagnetization**
- Computation in deformed unit cell
- $H_d$ jumps on particle boundaries

Actual energy computed by integration by parts
Energy evaluation: **Boundary Element Method**

**Elasticity in Grains**
- Full elastic subproblem via BEM
- Affine-periodic boundary of non-quadratic cell
- Force balance on **grain boundaries** with different lattice orientations
- Jump in eigenstrain
- Different fundamental solutions
- Handling of junction points
Energy evaluation: **Boundary Element Method**

**Elasticity in Grains**
- Full elastic subproblem via BEM
- Affine-periodic boundary of non-quadratic cell

Force balance on **grain boundaries** with different lattice orientations
- Jump in eigenstrain
- Different fundamental solutions
- Handling of junction points

**Demagnetization** as above
Results

Polycrystals versus Composites

2°  8°  ~ 20° (random)  misorientation
Polycrystals versus Composites

2°  8°  ~ 20° (random)  misorientation
Polycrystals versus Composites

- $2^\circ$ with 6% strain
- $8^\circ$ with 4% strain
- $\sim 20^\circ$ (random) misorientation with 2% strain

- 4% strain
Polycrystals versus Composites

2° close to single crystal

8° 4% strain

~ 20° (random) misorientation

6% 4% 2% strain

4% 4% 3% strain
Polycrystals versus Composites

2° close to single crystal
4% strain

8° 4% strain

~ 20° (random) misorientation
2% strain

accommodation of incompatibilities
4% strain

3% strain
Exploring Configurations

- Simple lattice, one particle in the periodic unit cell
- Plot work output for horizontally applied external magnetic field
Exploring Configurations

Simple lattice, one particle in the periodic unit cell
Plot work output for horizontally applied external magnetic field
Modify aspect ratio of particles

Particle Shape

![Particle Shapes](image)

![Graph](image)

Work Output in MPa vs. Aspect Ratio

- E = 6 GPa
- E = 1.2 GPa

Polymer Elastic Modulus in MPa

- ν = 0.49
- ν = 0.48
- ν = 0.45
- ν = 0.40
- ν = 0.25
Simple lattice, one particle in the periodic unit cell
Plot work output for horizontally applied external magnetic field
Modify orientation of particles

Particle Shape & Orientation,

- Work Output in MPa vs. Aspect Ratio
- Work Output in MPa vs. Rotation

- E = 6 GPa
- E = 1.2 GPa

Polymer Elastic Modulus in MPa

- \( \nu = 0.49 \)
- \( \nu = 0.48 \)
- \( \nu = 0.45 \)
- \( \nu = 0.40 \)
- \( \nu = 0.25 \)
Exploring Configurations

Simple lattice, one particle in the periodic unit cell
Plot work output for horizontally applied external magnetic field
Modify polymer elastic modulus and Poisson's ratio

Particle Shape & Orientation, Polymer Elasticity

- Plot work output for horizontally applied external magnetic field
- Modify polymer elastic modulus and Poisson's ratio
- Explore configurations with different aspect ratios and polymer elastic moduli
Demagnetization field

$$\int |\nabla \psi|^2 = \int |\nabla \psi_{\text{micro}}|^2 + \int |\nabla \psi_{\text{macro}}|^2$$

(Up to now only $\psi_{\text{micro}}$)

Can macroscopic part $\psi_{\text{macro}}$ induce additional scales?
Demagnetization field

\[ \int |\nabla \psi|^2 = \int |\nabla \psi_{\text{micro}}|^2 + \int |\nabla \psi_{\text{macro}}|^2 \]

(Up to now only \( \psi_{\text{micro}} \))

Can macroscopic part \( \psi_{\text{macro}} \) induce additional scales?

Analytical computation of \( \psi_{\text{macro}} \) for circular domain
Modeling Equilibrium Configurations  ➤ Results

Multiple Scales in the Magnetization

Demagnetization field

\[ \int |\nabla \psi|^2 = \int |\nabla \psi_{\text{micro}}|^2 + \int |\nabla \psi_{\text{macro}}|^2 \]

(Up to now only \( \psi_{\text{micro}} \))

Can macroscopic part \( \psi_{\text{macro}} \) induce additional scales?

Analytical computation of \( \psi_{\text{macro}} \) for circular domain

Compute cell with 4 particles to allow larger periodicity
No external field

- Average magnetization zero
- $\psi_{\text{macro}} = 0$, favored by $E_{\text{demag}}$
**Demagnetization and External Field**

- **Strong external field**
- Aligned magnetization, favored by $E_{\text{ext}}$
Modeling Equilibrium Configurations

Results

Additional Periodicity Scales

Intermediate stage (b) between zero-average and fully-aligned magnetization
Further length scales possible?  
Try larger computational cell
Some additional configurations in the phase diagram.
Rate-Independent Dynamics

Motion of Twin Boundaries

Moving Twin Boundaries in Changing External Field
Change in external field slow

\[\leadsto\] Rate independent model [Mielke et al.] without inertia terms, energy generated is completely dissipated

Why model the process as rate-independent?

\[\leadsto\] 1D example
Mass point moving in an oscillating potential with \textit{slow external forcing}

\[ m\ddot{x} = -\gamma \dot{x} + \kappa (vt - x) + a \cos(n\pi x) \]

\text{acceleration} \quad \text{friction} \quad \text{external forcing} \quad \text{periodic potential}
Equations of Motion

Mass point moving in an oscillating potential with *slow external forcing*

\[ m\ddot{x} = -\gamma \dot{x} + \kappa (vt - x) + a \cos(n\pi x) \]

Compute **energy differences** by integrating \( \int_0^\tau \ldots \dot{x} \, dt \) over **periodic interval** \([0; \tau]\) with \( x(\tau) = x(0) + 2/n, \dot{x}(\tau) = \dot{x}(0) \)

\[
\left. \frac{1}{2} m(\dot{x})^2 \right|_0^\tau = -\gamma \int_0^\tau (\dot{x})^2 \, dt + \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt - \mathcal{E}(t, x(t)) \right|_0^\tau
\]

with potential \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{n\pi} \sin(n\pi x) \)
\[
\frac{1}{2} m \dot{x}^2 \bigg|_0^\tau = - \gamma \int_0^\tau \dot{x}^2 \, dt + \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt - \mathcal{E}(t, x(t)) \bigg|_0^\tau
\]

with potential \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{n\pi} \sin(n\pi x) \)
Energy on Slow Timescale

\[ \frac{1}{2} m \dot{x}^2 \Bigg|_0^\tau = -\gamma \int_0^\tau (\ddot{x})^2 \, dt + \int_0^\tau \partial_t E(t, x(t)) \, dt - E(t, x(t)) \Bigg|_0^\tau \]

with potential \( E(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{n\pi} \sin(n\pi x) \)

\[ \frac{1}{2} m \dot{x}^2 \Bigg|_0^\tau = -\gamma \int_0^\tau (\ddot{x})^2 \, dt + \int_0^\tau \partial_t E(t, x(t)) \, dt - E(t, x(t)) \Bigg|_0^\tau \]

with potential \( E(t, x) = \frac{1}{2} \kappa (vt - x)^2 \)

since \( \sin(n\pi x(0)) = \sin(n\pi x(\tau)) \)
\[
\frac{1}{2} m(\dot{x})^2 \bigg|_0^\tau = -\gamma \int_0^\tau (\dot{x})^2 \, dt + \int_0^\tau \partial_t E(t, x(t)) \, dt - E(t, x(t)) \bigg|_0^\tau
\]

with potential \( E(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{n\pi} \sin(n\pi x) \)

\[
0 = -\gamma \int_0^\tau (\dot{x})^2 \, dt + \int_0^\tau \partial_t E(t, x(t)) \, dt - E(t, x(t)) \bigg|_0^\tau
\]

with potential \( E(t, x) = \frac{1}{2} \kappa (vt - x)^2 \)

since \( \dot{x}(0) = \dot{x}(\tau) \)
Energy on Slow Timescale

\[ \frac{1}{2} m(\dot{x})^2 \bigg|_{0}^{\tau} = -\gamma \int_{0}^{\tau} (\dot{x})^2 \, dt + \int_{0}^{\tau} \partial_t \mathcal{E}(t, x(t)) \, dt - \mathcal{E}(t, x(t)) \bigg|_{0}^{\tau} \]

with potential \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{n\pi} \sin(n\pi x) \)

\[ 0 = -\gamma D + \int_{0}^{\tau} \partial_t \mathcal{E}(t, x(t)) \, dt - \mathcal{E}(t, x(t)) \bigg|_{0}^{\tau} \]

with potential \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 \)

**Scale separation**, external force slow \( \sim \) energy completely dissipated on fast time scale, cf. damped harmonic oscillator

\[ \int_{0}^{\tau} (\dot{x})^2 \, dt \approx \int_{0}^{\infty} (\dot{x})^2 \, dt \approx \int_{0}^{\infty} C \left( \exp(-\frac{\gamma}{m} t) \sin(\omega t) \right)^2 \, dt \approx D \]
Energy on Slow Timescale

\[
\left. \frac{1}{2} m (\dot{x})^2 \right|_0^\tau = -\gamma \int_0^\tau (\dot{x})^2 \, dt + \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt - \mathcal{E}(t, x(t)) \bigg|_0^\tau
\]

with potential \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{\pi} \sin(n \pi x) \)

\[
\mathcal{E}(\tau, x(\tau)) + \gamma D = \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt + \mathcal{E}(0, x(0))
\]

new energy  
dissipated energy  
energy added  
old energy

with potential \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 \)
For one energy well

\[ \mathcal{E}(\tau, x(\tau)) + \gamma D \]

\[ = \mathcal{E}(0, x(0)) + \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt \]
Energy Dissipation: Rate-Independent Model

For one energy well

$$\mathcal{E}(\tau, x(\tau)) + \gamma D = \mathcal{E}(0, x(0)) + \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt$$

1–homogeneous in number of wells: $\mathcal{D}(x, \tilde{x}) = \gamma D \frac{2}{n} |x - \tilde{x}|$
For one energy well

\[ \mathcal{E}(\tau, x(\tau)) + \gamma D \]

\[ = \mathcal{E}(0, x(0)) + \int_0^\tau \partial_t \mathcal{E}(t, x(t)) \, dt \]

1–homogeneous in number of wells: \( \mathcal{D}(x, \tilde{x}) = \gamma D^{\frac{2}{n}} |x - \tilde{x}| \)

\[ \mathcal{E}(t, x(t)) + \mathcal{D}(x(0), x(t)) = \mathcal{E}(0, x(0)) + \int_0^t \partial_t \mathcal{E}(s, x(s)) \, ds \]

\[ \mathcal{E}(t, x(t)) \leq \mathcal{D}(x(t), \xi) + \mathcal{E}(t, \xi) \quad \forall \xi \]
For one energy well

\[ E(\tau, x(\tau)) + \gamma D \]

\[ = E(0, x(0)) + \int_0^\tau \partial_t E(t, x(t)) \, dt \]

1–homogeneous in number of wells:  \( D(x, \tilde{x}) = \gamma D_n^2 |x - \tilde{x}| \)

\[ E(t, x(t)) + D(x(0), x(t)) = E(0, x(0)) + \int_0^t \partial_t E(s, x(s)) \, ds \]

\[ E(t, x(t)) \leq D(x(t), \xi) + E(t, \xi) \quad \forall \xi \]

Implicit time discretization for  \( t = \tau, 2\tau, 3\tau, \ldots \)

\[ x(t) \text{ is minimizer of } E(t, x(t)) + D(x(t - \tau), x(t)) \]
Analogies to example
Wells ≈ Single atoms switching? No, timescale too slow
Dissipation Model

Analogy to example
Wells $\approx$ Single atoms switching? No, timescale too slow
Wells $\approx$ Interface traveling from one defect to the next

[Image: Likhachev and Ullakko 2000]

Uniform distribution of defects $\Rightarrow$ Dissipation proportional to volume switched

$$D(p, \tilde{p}) = \int_{\omega} |p - \tilde{p}|,$$

$p$ phase index
Analogy to example
Wells \(\approx\) Single atoms switching? No, timescale too slow
Wells \(\approx\) Interface traveling from one defect to the next

Uniform distribution of defects
\(\sim\) Dissipation proportional to volume switched

\[
D(p, \tilde{p}) = D \int_{\omega} |p - \tilde{p}|, \quad p \text{ phase index}
\]
Rate-Independent Dynamics  ➤  Modeling Twin Boundary Motion

Estimation of Dissipation Constant

\[ \mathcal{E}(t, x(t)) + \mathcal{D}(x(0), x(t)) = \mathcal{E}(0, x(0)) + \int_0^t \partial_t \mathcal{E}(s, x(s)) \, ds \]

\[ \mathcal{D}(p, \tilde{p}) = D \int_\omega |p - \tilde{p}|, \quad p \text{ phase index} \]

Estimate \( D \)?
Estimation of Dissipation Constant

\[
\mathcal{E}(t, x(t)) + D(x(0), x(t)) = \mathcal{E}(0, x(0)) + \int_{0}^{t} \partial_t \mathcal{E}(s, x(s)) \, ds
\]

\[
D(p, \tilde{p}) = D \int_{\omega} |p - \tilde{p}|, \quad p \text{ phase index}
\]

Estimate \( D \)? Consider switching in a single crystal

Energy gain by switching magnetization (from \( \mathcal{E}_{\text{ext}} \))

\[-M_s/\mu_0 \approx 0.5 \text{ M Pa/T per unit volume}\]

For minimal switching field of approximately 0.25 T, this balances with dissipation per unit volume

\[
D \approx 0.125 \text{ M Pa}
\]
Hysteresis Loops for Different Configurations
Hysteresis Loops for Different Configurations
Hysteresis Loops for Different Configurations
Hysteresis Loops for Different Configurations
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Hysteresis Loops for Different Configurations
Hysteresis Loops for Different Configurations

Hysteresis loop (preliminary numerics)
Twin Boundary Motion: Example
Twin Boundary Motion: Example

Thank You for Your Attention!

http://numod.ins.uni-bonn.de/people/lenz