A6: Mathematical Modeling and Simulation of Microstructured Magnetic-Shape-Memory Materials

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Polycrystals and Composites

**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**

cf. B8: O. Gutfleisch et al.
Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{ext}} + E_{\text{demag}} + E_{\text{exch}} + E_{\text{anis}} + E_{\text{elast}} + E_{\text{polymer}} \]

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

- \( \Omega \subset \mathbb{R}^d \) area occupied by composite
- \( \omega \subset \Omega \) area occupied by particles
- \( \omega = \Omega \) for polycrystals
- \( Q \) lattice orientation
- \( \nu \) deformation
- \( m \) magnetization
- \( p \) phase index
Model for Micromagnetism and Elasticity

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

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Interaction with External Field
Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{ext}} + E_{\text{demag}} + E_{\text{exch}} + E_{\text{anis}} + E_{\text{elast}}^{\text{MSM}} + E_{\text{elast}}^{\text{polymer}} \]

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

Demagnetization

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Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{ext}} + E_{\text{demag}} + E_{\text{exch}} + E_{\text{anis}} + E_{\text{elast, MSM}} + E_{\text{elast, polymer}} \]

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Magnetic Exchange
Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{ext}} + E_{\text{demag}} + E_{\text{exch}} + E_{\text{anis}} + E_{\text{elast}}^{\text{MSM}} + E_{\text{elast}}^{\text{polymer}} \]

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

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Anisotropy
Model for Micromagnetism and Elasticity

\[ E[v, m, p] = E_{\text{ext}} + E_{\text{demag}} + E_{\text{exch}} + E_{\text{anis}} + E_{\text{elast}}^{\text{MSM}} + E_{\text{elast}}^{\text{polymer}} \]

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

\[ \Omega \subset \mathbb{R}^d \quad \text{area occupied by composite} \]
\[ \omega \subset \Omega \quad \text{area occupied by particles} \]
\[ \omega = \Omega \quad \text{for polycrystals} \]
\[ Q \quad \text{lattice orientation} \]
\[ v \quad \text{deformation} \]
\[ m \quad \text{magnetization} \]
\[ p \quad \text{phase index} \]

**Particle / Grain Elasticity**

distance from phase-dependent eigenstrain
Model for Micromagnetism and Elasticity

\[
E[v, m, p] = E_{\text{ext}} + E_{\text{demag}} + E_{\text{exch}} + E_{\text{anis}} + E_{\text{elast\,MSM}} + E_{\text{elast\,polymer}}
\]

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

\(\Omega \subset \mathbb{R}^d\) area occupied by composite
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\(Q\) lattice orientation
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**Matrix Elasticity**
*(only in composites)*
Consider periodicity cell with several particles: **stepwise switching** of magnetization

![Diagram of energy density and external field](image)
Simulation Results

Experimental Observation

Significantly softer polymer needed

B8: O. Gutfleisch et al.

Polyester $\sim 100$ MPa

Polyurethane $\sim 10$ MPa
Simulation Results

Experimental Observation
Significantly softer polymer needed

B8: O. Gutfleisch et al.
Polyester $\sim$ 100 MPa
Polyurethan $\sim$ 10 MPa
Microstructure of Twins and Magnetic Domains
Description of effective behaviour by relaxation theory: appropriate convex envelope (cross-quasiconvexity)

Twins in MSM Particle
(B8: O. Gutfleisch et al.)
Proposed Solution: Modelling Large Particles

Microstructure of Twins and Magnetic Domains
Description of effective behaviour by relaxation theory: appropriate convex envelope (cross-quasiconvexity)

First Approximation: Convex Envelope
For the magnetic anisotropy (for $|m| = 1$ and $p \in \{0; 1\}$)

$$\gamma(p, m) = \begin{cases} m_2^2 & : p = 0, \\ m_1^2 & : p = 1, \end{cases}$$

the convex envelope (for $|m| \leq 1$ and $p \in [0; 1]$) is

$$\gamma_{\text{conv}}(p, m) = \begin{cases} 0 & : |m_1| \leq 1 - p \wedge |m_2| \leq p, \\ \frac{(|m_2| - p)^2}{1-p} & : |m_1| \leq \sqrt{(1 - |m_2|)(1 + |m_2| - 2p)}, \\ \frac{(|m_1| - 1 + p)^2}{p} & : |m_2| \leq \sqrt{(1 - |m_1|)(2p + |m_1| - 1)}, \\ p \sqrt{\sin(\sin^{-1}\frac{|m_1|}{|m|} - \cos^{-1}\frac{|m_2| - 1 + 2p}{2p|m|})} & : |m_1| \leq 1 - p \wedge |m_2| \leq p, \\ (1-p) \sqrt{\cos(\cos^{-1}\frac{|m_2|}{|m|} + \cos^{-1}\frac{|m_2| - 1 - 2p}{2(1-p)|m|})} & : \text{else.} \end{cases}$$
Simulation of Large Particles

Good Agreement with Experiments

Measurement

Simulation

B8: O. Gutfleisch et al.

preliminary numerics
Simulation of Large Particles

Good Agreement with Experiments

Measurement

Simulation

B8: O. Gutfleisch et al.

Planned Research

- Identify appropriate convex envelope
- Systematic simulations: comparison to experiments, guide material production
Tool: Rate Independent Modeling

Simulation of cell problem
Hysteresis & Twin Boundary Motion

Tool: Rate Independent Modeling
Hysteresis & Twin Boundary Motion

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Hysteresis & Twin Boundary Motion

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Hysteresis & Twin Boundary Motion

Tool: Rate Independent Modeling

Hysteresis loop (preliminary numerics)

Magnetization in a.u.
External Field in T

A
B
Twin Boundary Motion: Example

Planned Research

Polycrystals

Combination of relaxation with the evolutionary model

Geometric criteria for continuous switching
Twin Boundary Motion: Example

Planned Research

- Polycrystals
- Combination of relaxation with the evolutionary model
- Geometric criteria for continuous switching
Cooperations & Connections within the Program

B8: Polymer Bonded Textured Composites (O. Gutfleisch)
- Modeling based on experimental observations
- Large particles \( \rightarrow \) relaxation
- Improvement of material production based on theory
- Composite geometry and twin boundary motion

B9: MSM for Vibration Damping (H. Janocha)
- Homogeneous switching

A7: Continuum Models for MSM Materials (S. Müller, F. Otto)
- Continuum modeling across scales
- Mathematical techniques

A5: Phase Field Modeling of Microstructure Evolution (B. Nestler)
- Modeling with phase fields