Modeling and Simulation of Twin Boundary Motion in Magnetic-Shape-Memory Composites

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Supported by DFG SPP 1239

March 23rd, 2010
Magnetic Shape Memory Materials

E.g. **NiMnGa**
deforms in magnetic field,
Ullakko et al. (1996)

- Fast switching
  \[ \approx 10^3 \text{Hz} \]
- Large deformation
  \[ \approx 10\% \]
- Large work output
  \[ \approx 10^5 \text{Pa} \]

Lai, McCord (IFW Dresden)

\[\rightsquigarrow\text{ Actuators and Sensors}\]
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Lai, McCord (IFW Dresden)
Introduction

Magnetic Shape Memory Composites

Polycrystals incompatibilities at grain boundaries

Composites with polymer matrix, cf. Gutfleisch (IFW Dresden)

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
Modeling Twin Boundary Motion

Two-Dimensional Model of the Phase Transformation

Martensitic Variants

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

Anisotropy for the Magnetization

\[
m_\gamma_1 (m) = m, \quad m_\gamma_2 (m) = m
\]
Modeling Twin Boundary Motion

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\]

Linearized Elastic Transformation Strain

Anisotropy for the Magnetization

\[ m_1^{\gamma} = m_2^{\gamma_2} \]

\[ m_2^{\gamma_2} = m_2^{\gamma_2} \]
Martensitic Variants

Linearized Elastic Transformation Strain

\[ \bar{\varepsilon}_1 = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & -\varepsilon_0 \end{pmatrix} \]
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Anisotropy for the Magnetization \( m \)

\[ \gamma_1(m) = m_1^2 \]
\[ \gamma_2(m) = m_2^2 \]
Modeling Twin Boundary Motion

Static Model combining Micromagnetism and Elasticity

\[ \mathcal{E}[\nu, m, p] = \mathcal{E}_{\text{polymer}} + \mathcal{E}_{\text{elast}} + \mathcal{E}_{\text{MSM}} + \mathcal{E}_{\text{ext}} + \mathcal{E}_{\text{demag}} + \mathcal{E}_{\text{anis}} + \mathcal{E}_{\text{exch}} \]

\[ \Omega \subset \mathbb{R}^2 \]  
area occupied by composite

\[ \omega \subset \Omega \]  
area occupied by particles

\[ \nu : \Omega \to \mathbb{R}^2 \]  
elastic deformation

\[ m : \nu(\omega) \to \mathbb{R}^2 \]  
magnetization

\[ p : \omega \to \{1, 2\} \]  
phase / variant parameter

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

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

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

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

\[ + \int_{\nu(\omega)} \gamma_p((RQ)^T m) \]

\[ + \int_{\nu(\omega)} \frac{1}{2} d^2 |\nabla m|^2 \]
**Modeling Twin Boundary Motion**

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**Matrix Elasticity**

\[ W_{\text{polymer}} \]

stored energy density of polymer bulk

\[ \nu : \Omega \rightarrow \mathbb{R}^2 \]

deformation
Modeling Twin Boundary Motion

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phase / variant parameter

Particle Elasticity

\[ W_{\text{MSM}} \]

stored energy density of MSM particles, i.e. quadratic distance to transformation strain \( \bar{e}_p \) with respect to crystal lattice orientation

\[ Q : \omega \rightarrow SO(2) \]

crystal lattice orientation
Modeling Twin Boundary Motion

Static Model combining Micromagnetism and Elasticity

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

\[ \Omega \subset \mathbb{R}^2 \quad \text{area occupied by composite} \]
\[ \omega \subset \Omega \quad \text{area occupied by particles} \]
\[ v : \Omega \rightarrow \mathbb{R}^2 \quad \text{elastic deformation} \]
\[ m : v(\omega) \rightarrow \mathbb{R}^2 \quad \text{magnetization} \]
\[ p : \omega \rightarrow \{1, 2\} \quad \text{phase / variant parameter} \]

Interaction with External Field

\[ H_{\text{ext}} \in \mathbb{R}^2 \quad \text{external magnetic field} \]
Static Model combining Micromagnetism and Elasticity

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

Demagnetization

\[ H_d : \mathbb{R}^2 \rightarrow \mathbb{R}^2 \quad \text{demagnetization field} \]

\[ H_d = \nabla \psi \]

\[ \Delta \psi = \text{div} \ m \quad \text{distributionally} \]
Modeling Twin Boundary Motion

Static Model combining Micromagnetism and Elasticity

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- \( \omega \subset \Omega \) area occupied by particles
- \( v : \Omega \rightarrow \mathbb{R}^2 \) elastic deformation
- \( m : v(\omega) \rightarrow \mathbb{R}^2 \) magnetization
- \( p : \omega \rightarrow \{1, 2\} \) phase / variant parameter

Anisotropy

\( \gamma_p : \mathbb{R}^2 \rightarrow \mathbb{R} \) anisotropy in phase \( p \)

- \( R \in SO(2) \) rotational part of deformation \( \nabla v = RU \)
- \( Q : \omega \rightarrow SO(2) \) crystal lattice orientation
Modeling Twin Boundary Motion

Static Model combining Micromagnetism and Elasticity

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Magnetic Exchange
\[ m : \nu(\omega) \to \mathbb{R}^2 \quad \text{magnetization} \]
Slowly changing external field
\[ \Rightarrow \text{rate-independent model without inertia terms} \]

- \( \mathcal{E}(t, x) \) Energy of configuration \( x \) at time \( t \)
- \( \mathcal{D}(\dot{x}) \) Energy dissipated moving with velocity \( \dot{x} \)
Slowly changing external field

Θ rate-independent model without inertia terms

- \( E(t, x) \) Energy of configuration \( x \) at time \( t \)
- \( D(\dot{x}) \) Energy dissipated moving with velocity \( \dot{x} \)

\[
E(t, x(t)) + \int_0^t D(\dot{x}(s)) \, ds = E(s, x(s)) + \int_0^t \partial_t E(s, x(s)) \, ds
\]
Slowly changing external field
\[ \xrightarrow{\sim} \text{rate-independent model without inertia terms} \]
- \( \mathcal{E}(t, x) \): Energy of configuration \( x \) at time \( t \)
- \( \mathcal{D}(\dot{x}) \): Energy dissipated moving with velocity \( \dot{x} \)

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\]

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

\[ x(t + \tau) \quad \text{is minimizer of} \quad \mathcal{E}(t + \tau, x) + \mathcal{D}(x - x(t)) \]
**Rate-Independent Model for Twin Boundary Motion**

**Slowly changing external field**

$\leadsto$ rate-independent model without inertia terms

- $\mathcal{E}(t, x)$ Energy of configuration $x$ at time $t$
- $\mathcal{D}(\dot{x})$ Energy dissipated moving with velocity $\dot{x}$

\[
\mathcal{E}(t, x(t)) + \int_0^t \mathcal{D}(\dot{x}(s)) \, ds = \mathcal{E}(s, x(s)) + \int_0^t \partial_t \mathcal{E}(s, x(s)) \, ds
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x(t + \tau) \quad \text{is minimizer of} \quad \mathcal{E}(t + \tau, x) + \mathcal{D}(x - x(t))
\]

**Dissipation** proportional to volume switched

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

Small, Rigid Particles and Homogenization

- Particles are small and hard
  - \( \Rightarrow \) particle deformations are affine
- Particles are single crystals
  - \( \Rightarrow \) lattice orientation \( Q \) constant on each particle

Homogenization

\( E_{\text{exch}} \sim \text{length of twin boundary} \)
Particles are small and hard
   \[\rightsquigarrow \text{particle deformations are affine}\]

Particles are single crystals
   \[\rightsquigarrow \text{lattice orientation } Q \text{ constant on each particle}\]

One planar twin boundary per particle
   \[\rightsquigarrow \text{phase } p \text{ constant on each side}\]

No additional magnetic domain walls
   \[\rightsquigarrow \text{magnetization } m \text{ constant in each twin}\]
   \[\rightsquigarrow E_{\text{exch}} \sim \text{length of twin boundary}\]
- Particles are small and hard
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  \(\Rightarrow\) lattice orientation \(Q\) constant on each particle

- One planar twin boundary per particle
  \(\Rightarrow\) phase \(p\) constant on each side

- No additional magnetic domain walls
  \(\Rightarrow\) magnetization \(m\) constant in each twin
  \(\Rightarrow\) \(E_{\text{exch}}\) \(\sim\) length of twin boundary

- Deformations are (relatively) small
  \(\Rightarrow\) linearized elasticity

- Homogenization
  \(\Rightarrow\) study periodic configurations
Minimize over internal variables

- particle deformation on each side
- twin boundary position
- twin magnetizations
Minimize over internal variables

- particle deformation on each side $8$
- twin boundary position $2$
- twin magnetizations $1+1$

12 degrees of freedom per particle
Minimize over internal variables

- particle deformation on each side 8
- twin boundary position 2
- twin magnetizations 1+1

12 degrees of freedom per particle

- Energy minimization
  \[\leadsto\] Gradient Descent
- Gradient approximation
  \[\leadsto\] Finite Differences
- Energy evaluation
  (elasticity and stray field)
  \[\leadsto\] Boundary Elements
Problem: Inserting and moving the triple points between twin boundary and particle boundary adds *spurious oscillations* to Boundary Element solution, and thus to the discrete energy.
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**Ansatz:** Do not insert triple point. Boundary values depend on distance from twin boundary: *Regularize* distance to make energy *differentiable*.
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Numerical Approximation

Regularity of Discrete Energy

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**Implementation for full model:** Polymer elasticity.

\[ h = \varepsilon = 0.1 \]

\[ h = \varepsilon = 0.025 \]

![Graph of Elastic Energy vs. Position of Twin Boundary for different cases](image1)

![Graph of Elastic Energy vs. Position of Twin Boundary for different cases](image2)
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---

**Similar Regularization** for Dissipation \( \mathcal{D} \)
Results

Twin Boundary Motion & Hysteresis

Macroscopic Strain in x-direction in %

External Field in T

(1) Field in y-direction

E = 2.8 MPa
Twin Boundary Motion & Hysteresis

Results

Macroscopic Strain in x-direction in %

External Field in T

(2): Field in x-direction

(1)        : Field in y-direction

E = 2.8 MPa
Results

Twin Boundary Motion & Hysteresis

-3
-2
-1
0
1
2
3
-1 -0.5 0 0.5 1

Macroscopic Strain in x-direction in %

External Field in T

(2): Field in x-direction

(1) + (3): Field in y-direction

E = 2.8 MPa
**Results**

**Twin Boundary Motion & Hysteresis**

- **Macroscopic Strain in x-direction in %**
- **External Field in T**

- **(2): Field in x-direction**
- **(1) + (3): Field in y-direction**

- **E = 1.4 MPa**
- **E = 2.8 MPa**
Results

Twin Boundary Motion

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