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

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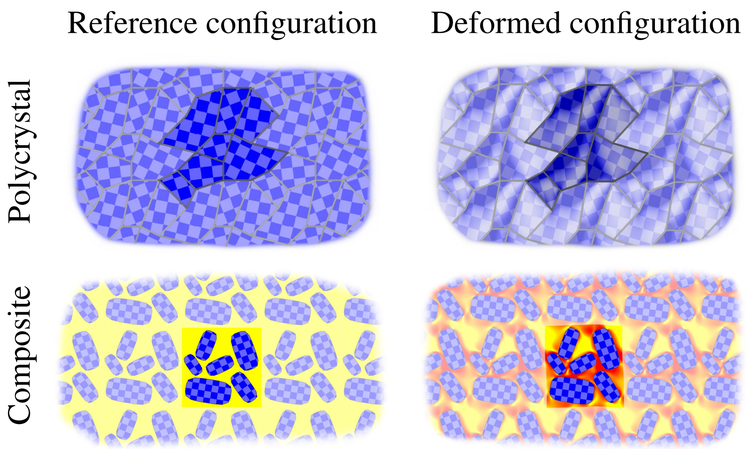
## 1 Introduction




## 2 Micromagnetic-Elastic Model

$\Omega$ material domain — $p$ phase index
$\omega, \omega_i$ grains / particles — $Q$ lattice orientation

**Elasticity.**

$$E^{\mathrm{MSM}}_{\mathrm{elast}} = \int_\omega W^{\mathrm{MSM}}((\nabla v(x))Q(x) - \varepsilon_{p(x)})\,dx$$

$$\varepsilon_1 = \begin{pmatrix} -\varepsilon_0 & 0 \\ 0 & \varepsilon_0 \end{pmatrix}, \quad \varepsilon_2 = \begin{pmatrix} \varepsilon_0 & 0 \\ 0 & -\varepsilon_0 \end{pmatrix} \quad \text{eigenstrains}$$

$$E^{\mathrm{polymer}}_{\mathrm{elast}} = \int_{\Omega\setminus\omega} W^{\mathrm{polymer}}(\nabla v(x))\,dx$$

$u, v$ elastic displacement and deformation
$W^{\mathrm{MSM}}(F)$ cubic elastic energy density of MSM
$W^{\mathrm{polymer}}(F)$ isotropic elastic energy density of polymer

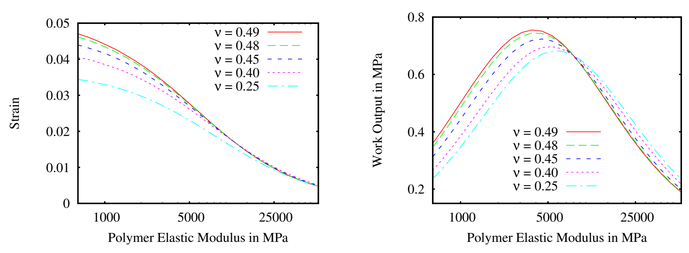
**Micromagnetism.**

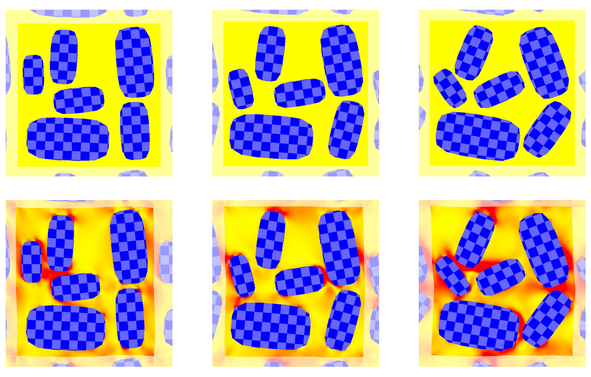
$$E_{\mathrm{demag}} = \frac{1}{2}\frac{M_s^2}{\mu_0}\int_{\mathbb{R}^2} |H_d|^2\,dy$$
$$E_{\mathrm{ext}} = -\frac{M_s}{\mu_0}\int_{\mathbb{R}^2} H_{\mathrm{ext}}\cdot m\,dy$$
$$E_{\mathrm{aniso}} = K_u \int_{v(\omega)} \varphi_{p(v^{-1}(y))}\left((R_{\nabla v\circ v^{-1}}Q(y))^T m\right)\,dy$$

$$\varphi_2(m) = m_1^2, \quad \varphi_1(m) = m_2^2 \quad \text{anisotropies}$$

$m$ magnetization — $H_{\mathrm{ext}}$ external field
$H_d$ stray field — $R_F$ rotational part of $F$

## 3 Simulation Results



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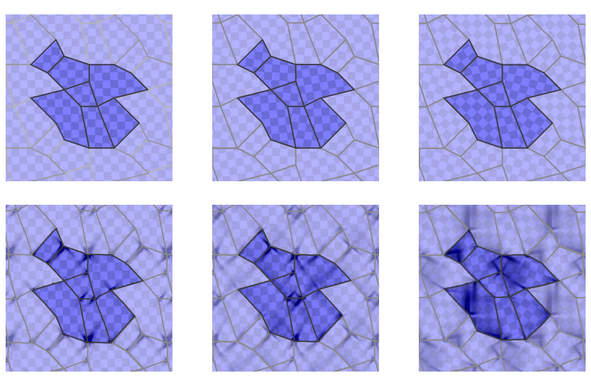
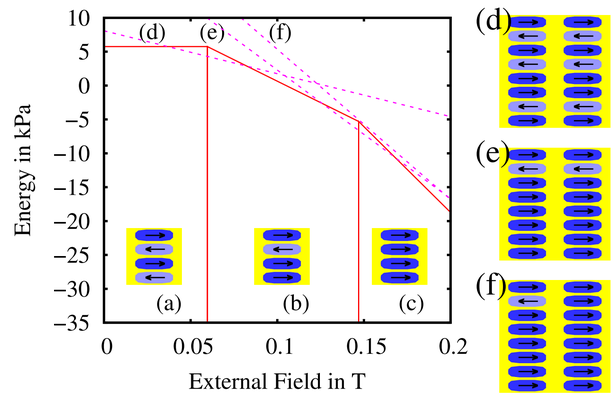


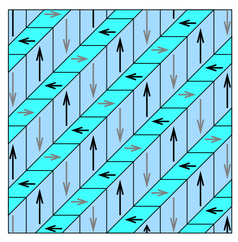
6 % 4 % 2 %

**Magnetization at different scales.**




## 4 Relaxation

Microstructure of twins and magnetic domains significantly smaller than particle / grain geometry: Compute only volume fraction of twin variants and average magnetization
⇝ **Relaxation theory**



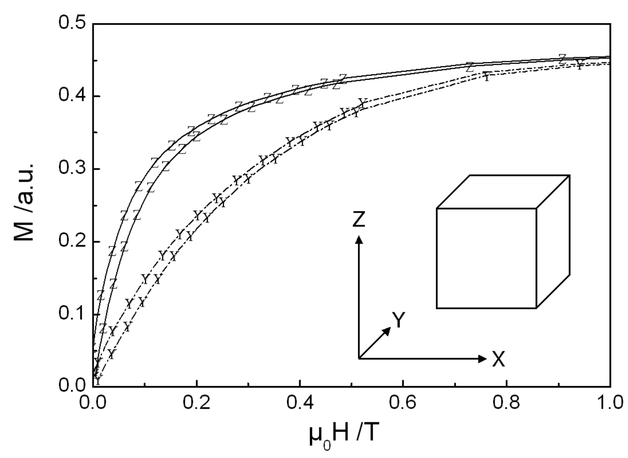
**Theorem.** Consider for $|m| = 1$ and $p \in \{0;1\}$ the anisotropy

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

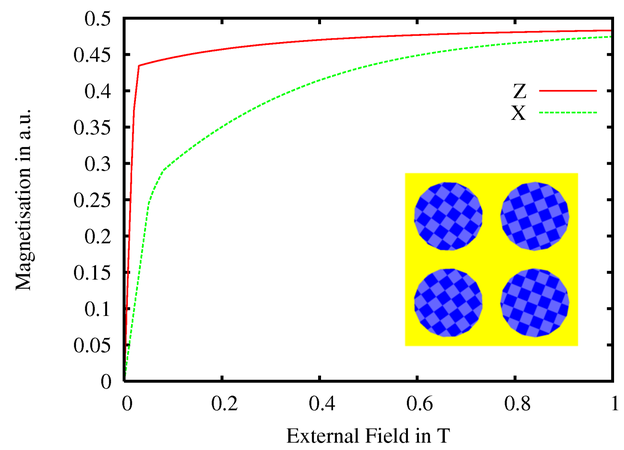
Then its convex envelope for $|m| \le 1$ and $p \in [0;1]$ is

$$\gamma^{\mathrm{conv}}(p,m) = \begin{cases} 0 & : |m_1| \le 1-p \wedge |m_2| \le p, \\ \frac{(|m_2|-p)^2}{1-p} & : |m_1| \le \sqrt{(1-|m_2|)(1+|m_2|-2p)}, \\ \frac{(|m_1|-1+p)^2}{p} & : |m_2| \le \sqrt{(1-|m_1|)(2p+|m_1|-1)}, \\ p\sqrt{\sin(\sin^{-1}\frac{|m_1|}{|m|} - \cos^{-1}\frac{|m|^2-1+2p}{2p|m|})} & \\ +(1-p)\sqrt{\cos(\cos^{-1}\frac{|m_2|}{|m|} + \cos^{-1}\frac{|m|^2+1-2p}{2(1-p)|m|})} & : \text{else.} \end{cases}$$

**Experiment by O. Gutfleisch et al.**




**Simulation: preliminary numerics**




**To Do:**
Explanation of the gap between experiments and previous simulations:

- rigorous derivation of the relaxed model (convex vs. quasiconvex envelope)
- identifying parameters from experiments

Systematic simulations: guide material production (with project B8, O. Gutfleisch)

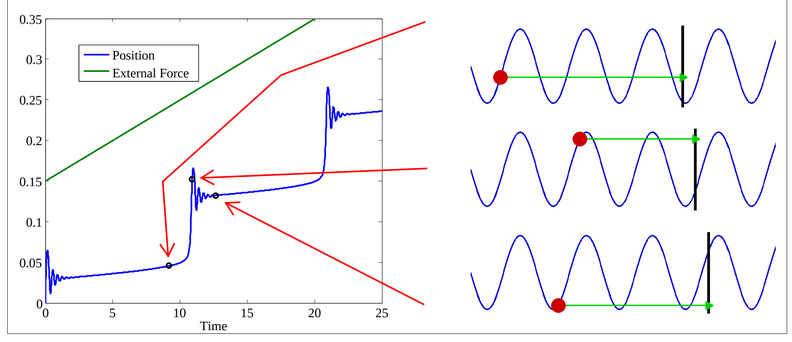
## 5 Rate-Independent Evolution

**Toy model.**
Slow external forcing, energy completely dissipated:

$$\mathscr{E}(t,x(t)) + \mathscr{D}(x(0),x(t)) = \mathscr{E}(0,x(0)) + \int_0^t \partial_t\mathscr{E}(s,x(s))\,ds$$

Implicit time discretization for $t = \tau, 2\tau, 3\tau, \ldots$:

$$x(t) \quad \text{is minimizer of} \quad \mathscr{E}(t,x(t)) + \mathscr{D}(x(t-\tau),x(t)))$$

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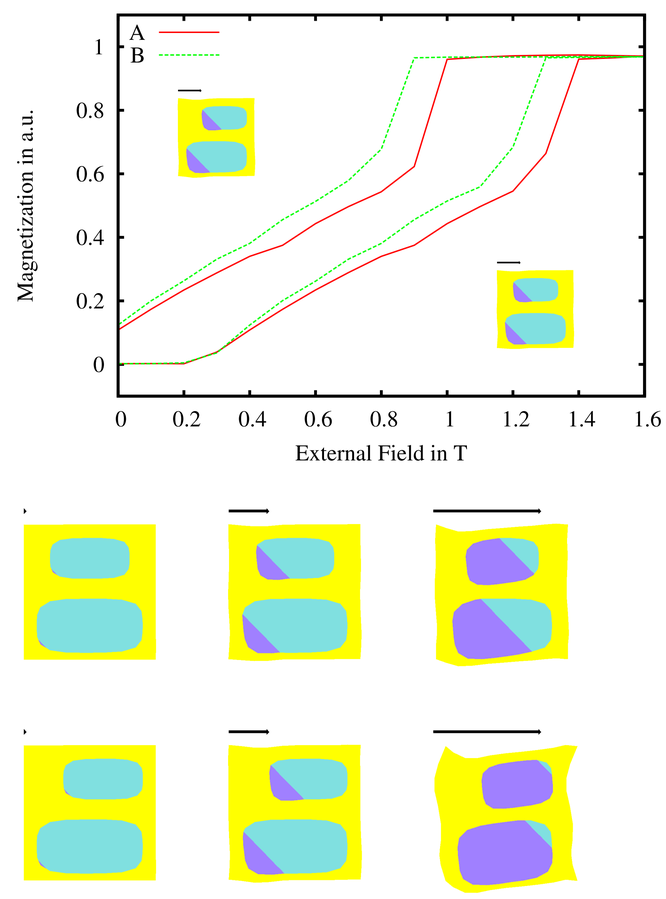


**To Do:**
- Inclusion of particle elasticity, magnetization modulation, and appropriate boundary conditions in the current simulation algorithm
- Polycrystals
- Large grain limit of the evolutionary model combining relaxation and hysteresis
- Systematic simulations: geometric criteria for continuous switching (with project B9, H. Janocha and B8, O. Gutfleisch)

## 6 Cooperations & Connections

**Project B8** *Polymer bonded textured composites with single crystalline $Ni_2MnGa$ particles for magnetic-field controlled dampers and actuators* (O. Gutfleisch).
- modeling based on experimental observations
- improvement of material production based on theory
- identification of length scales for relaxation approach
- effect of composite geometry on twin boundary motion

**Project A7** *Continuum models of magnetic shape memory materials: mathematics* (S. Müller, F. Otto).
- phase transitions at different time and length scales
- mathematical techniques for microstructured materials

**Project B9** *Magnetic Shape-memory alloys as active materials for vibration damping* (H. Janocha).
- design of composites with homogeneous switching

**Project A5** *Phase-field modelling of magnetically induced microstructure evolution in martensitic polycrystals* (B. Nestler).
- phase field models for martensitic microstructures