Mathematical Modeling and Simulation of Microstructured MSM Devices

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SPP 1239 Convention in Wesseling
on September 3rd – 6th, 2007
Overview

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Polycrystals and Composites

Microstructures in MSM Materials: Polycrystals and Composites
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**Polycrystals**
Incompatibilities at grain boundaries lead to smaller deformations
Microstructures in MSM Materials: Polycrystals and Composites

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**Composites**
Polymer matrix accommodates deformation of small particles
cf. project B8, Gutflieisch et al.
Microstructures in MSM Materials: Polycrystals and Composites

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**Polycrystals**

**Composites**

**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
Full Model for Micromagnetism and Elasticity

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

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

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

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

Full Model for Micromagnetism and Elasticity

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

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

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

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

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

\[ + \int_{v(\omega)} \varphi_p ((RQ)^T m) \]

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

\( \Omega \subset \mathbb{R}^d \) 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
### Full Model for Micromagnetism and Elasticity

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

- \( \Omega \subset \mathbb{R}^d \): 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

- \( p : \omega \rightarrow \{1, \ldots, d\} \): phase parameter in particles / grains
- \( Q : \omega \rightarrow SO(d) \): lattice orientation in particles / grains
- \( v : \Omega \rightarrow \mathbb{R}^d \): deformation

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

Full Model for Micromagnetism and Elasticity

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

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

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

Interaction with External Field

\( m : \nu(\omega) \rightarrow \mathbb{R}^d \) magnetization
\( H_{\text{ext}} \in \mathbb{R}^d \) external magnetic field
### Model Equilibirum Configurations

**Micromagnetic–Elastic Model**

**Full Model for Micromagnetism and Elasticity**

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

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

**Demagnetization**

- \(m : \mathbb{R}^d \to \mathbb{R}^d\) magnetization
- \(H_d : \mathbb{R}^d \to \mathbb{R}^d\) demagnetization field

\[
H_d = \nabla \psi \\
\Delta \psi = \text{div} m \quad \text{distributionally}
\]
**Full Model for Micromagnetism and Elasticity**

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

- **Anisotropy**
  - \( m : \nu(\omega) \to \mathbb{R}^d \) magnetization
  - \( p : \omega \to \{1, \ldots d\} \) phase parameter in particles / grains
  - \( \varphi_p : \mathbb{R}^d \to \mathbb{R} \) anisotropy in phase \( p \) applied to magnetization in deformed lattice
  - \( R \in \text{SO}(d) \) rotational part of deformation \( \nabla u = RU \)
  - \( Q : \omega \to \text{SO}(d) \) lattice orientation in particles / grains

\( \Omega \subset \mathbb{R}^d \) area occupied by composite

\( \omega \subset \Omega \) area occupied by particles

\( \omega = \Omega \) for polycrystals
Modeling Equilibrium Configurations ➞ Micromagnetic–Elastic Model

Full Model for Micromagnetism and Elasticity

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

\[ + E_{\text{MSM}}^{\text{elast}} \]

\[ + E_{\text{ext}} \]

\[ + E_{\text{demag}} \]

\[ + E_{\text{anis}} \]

\[ + E_{\text{exch}} \]

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

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

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

**Magnetic Exchange**

\[ m : v(\omega) \rightarrow \mathbb{R}^d \quad \text{magnetization} \]
Reduction to 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 / grain
- Particles / grains are single-domain
  - \( \Rightarrow \) phase \( p \) and magnetization \( m \) constant on particles / grains
  - \( \Rightarrow \) \( E_{\text{exch}} = 0 \)
- Deformations are (relatively) small
  - \( \Rightarrow \) linearized elasticity
- Large numbers of small particles or grains, Fully resolved simulation not feasible
  - \( \Rightarrow \) Homogenization: Study periodic configurations
Polycrystals versus Composites

2°  8°  ∼ 20° (random) misorientation
Modeling Equilibrium Configurations

Results

Polycrystals versus Composites

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

2°  8°  ~ 20° (random) misorientation

6%  4%  2% strain

4%  4%  3% strain
Modeling Equilibrium Configurations

Polycrystals versus Composites

2°
8°
≈ 20° (random) misorientation

close to single crystal

6%
4%
2% strain

4%
4%
3% strain
Modeling Equilibrium Configurations ➤ Results

Polycrystals versus Composites

2° close to single crystal

8° 4% strain

2° (random) misorientation

6% 4% 2% strain

accommodation of incompatibilities

4% 4% 3% strain
Polycrystals versus Composites

- 2° close to single crystal
- 8°
- ~ 20° (random) misorientation

6% strain
4% strain
2% strain

accommodation of incompatibilities

Effect of Polymer Elasticity

Plot strain and work output for different polymer elastic moduli.

\[ \text{Longer particles, (somewhat) softer polymer} \]

(In comparison: For particles is \( E \approx 100\,000 \, \text{MPa} \))
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
Influence of Macroscopic Demagnetization

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
**Demagnetization and External Field**

- **No external field**
  - Average magnetization zero
  - $\psi_{macro} = 0$, favored by $E_{demag}$
Demagnetization and External Field

- Strong external field
- Aligned magnetization, favored by $E_{\text{ext}}$
Intermediate stage (b) between zero-average and fully-aligned magnetization
Further length scales possible?
Try larger computational cell
Additional Periodicity Scales

Some additional configurations in the phase diagram
Twin Boundaries in Particles

Up to now: Particles / grains consist of one *single variant*

Next step: *One twin boundaries* in a particle
Twin Boundaries in Particles

Up to now: Particles / grains consist of one *single variant*

Next step: **One twin boundaries** in a particle

Possible directions of twin boundaries?
Deformation has to be continuous
\[ \nabla u \cdot \tau \text{ continuous for tangent } \tau \]
\[ \nabla_+ u - \nabla_- u = \nu \otimes \nu \text{ for normal } \nu \text{ and some } \nu \]
Up to now: Particles / grains consist of one **single variant**

Next step: **One twin boundaries** in a particle

Possible directions of twin boundaries?

Deformation has to be continuous

\[ \nabla u \cdot \tau \text{ continuous for tangent } \tau \]

\[ \nabla_+ u - \nabla_- u = \mathbf{v} \otimes \mathbf{v} \text{ for normal } \mathbf{v} \text{ and some } \mathbf{v} \]

Directions \( \mathbf{v} \) where \( Q \bar{\varepsilon}_1 - \bar{\varepsilon}_2 = \mathbf{v} \otimes \mathbf{v} \) for some \( Q \in SO(2) \)?
Up to now: Particles / grains consist of one single variant

Next step: One twin boundaries in a particle

Possible directions of twin boundaries?
Deformation has to be continuous
\[ \nabla u \cdot \tau \text{ continuous for tangent } \tau \]
\[ \nabla_+ u - \nabla_- u = \nu \otimes \nu \text{ for normal } \nu \text{ and some } \nu \]

Directions \( \nu \) where \( Q \bar{\varepsilon}_1 - \bar{\varepsilon}_2 = \nu \otimes \nu \) for some \( Q \in SO(2) \)?

\[ \nu = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ or } \nu = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \]
Moving twin boundaries with changing external field
Moving twin boundaries with changing external field

Change in external field slow

→ Rate independent model without inertia terms, energy generated is completely dissipated

Why model the process as rate-independent?

→ 1D example
Mass point moving in a periodic potential with **slow external forcing**

\[
\begin{align*}
\ddot{x} & = -\gamma \dot{x} + \kappa (vt - x) + a \cos(n\pi x) \\
\text{acceleration} & \quad \text{friction} \quad \text{external forcing} \quad \text{periodic potential}
\end{align*}
\]
Rate-Independent Modeling ➞ 1D Example

Equations of Motion

Mass point moving in a periodic potential with slow external forcing

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

acceleration, friction, external forcing, periodic potential

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

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

kinetic, friction, power, potential

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 \( \mathcal{E}(t, x) = \frac{1}{2} \kappa (vt - x)^2 - \frac{a}{n\pi} \sin(n\pi x) \)
Rate-Independent Modeling ➞ 1D Example

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

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

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

since \( \sin(n\pi x(0)) = \sin(n\pi x(\tau)) \)
Rate-Independent Modeling
1D Example

Energy on Slow Timescale

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

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 \( \dot{x}(0) = \dot{x}(\tau) \)
Rate-Independent Modeling

1D Example

Energy on Slow Timescale

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

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

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

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

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

\[ \int_0^\tau (\dot{x})^2 \, dt \approx \int_0^\infty (\dot{x})^2 \, dt \approx \int_0^\infty C \left( \exp\left(-\frac{\gamma}{m} t\right) \sin(\omega t) \right)^2 \, dt \approx D \]
Rate-Independent Modeling

1D Example

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

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

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

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

\[ = \mathcal{E}(0, x(0)) + \int_{0}^{\tau} \partial_t \mathcal{E}(t, x(t)) \, dt \]
For one energy well

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

**Dissipation is 1–homogeneous** in the number of wells traversed

\[ D(x, \tilde{x}) = \gamma D \frac{2}{n} |x - \tilde{x}| \]
For one energy well

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

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

**Dissipation is 1–homogeneous** in the number of wells traversed

\[ \mathcal{D}(x, \tilde{x}) = \gamma D \frac{2}{n} |x - \tilde{x}| \]

**Implicit time discretization**

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

\[ x(t) = \arg \min_{\xi} (\mathcal{E}(t, \xi) + \mathcal{D}(x(t - \tau), \xi)) \]
Dissipation Model

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

(Likhachev and Ullakko 2000)
Analogy to example
Wells ≈ Single atoms switching? No, timescale too slow
Wells ≈ Interface traveling from one defect to the next

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

Estimation of Dissipation Constant

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

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

Estimate \( D \)?
Estimation of Dissipation Constant

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

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

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

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

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

For minimal switching field of \( \approx 0.25 \text{ T} \), this balances with dissipation per unit volume

\[ D \approx 0.125 \text{ M Pa} \]
Motion of one interface by increasing $H_{\text{ext}}$
Simplified model, coarse numerics

![Graph showing stretch in % and external field in T against interface position.]

![Graph showing stored energy and dissipated energy against interface position.]}
Motion of one interface by increasing $H_{ext}$
Simplified model, coarse numerics
Rate-Independent Modeling  ➤  First Numerical Results

Motion of a Twin Boundary in a Particle

Motion of one interface by increasing $H_{\text{ext}}$

Simplified model, coarse numerics
Motion of one interface by increasing $H_{\text{ext}}$
Simplified model, coarse numerics
Motion of a Twin Boundary in a Particle

Motion of one interface by increasing $H_{\text{ext}}$
Simplified model, coarse numerics

![Graphs showing stretch in %, external field in T, stored energy, and dissipated energy as functions of interface position.](image-url)
Motion of one interface by increasing $H_{\text{ext}}$
Simplified model, coarse numerics
Motion of one interface by increasing $H_{ext}$
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Hysteresis
Interesting Questions

Nucleation: Tip or center?
Interesting Questions

Nucleation: Tip or center?

Effective $H_{\text{ext}}$ – strain - relation
Interesting Questions

Nucleation: Tip or center?

Effective $H_{\text{ext}}$ – strain - relation

http://analysis.math.uni-duisburg.de/research/spp1239.html