Mathematical and computational modelling of bulk ferromagnets

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Steady-state problem, a microscopical level:

(Landau and Lifshitz (1935), Brown (1962-66))

$$
\begin{cases}
\text{minimize} & E_\varepsilon(m,u) - \int_\Omega h\cdot m\,\mathrm{d}x \\
\text{where} & E_\varepsilon(m,u) := \int_\Omega \Big[\varphi(m) + \varepsilon|\nabla m|^2\Big]\,\mathrm{d}x \\
& \qquad + \frac{1}{2}\int_{\mathbb{R}^n} |\nabla u|^2\,\mathrm{d}x\ , \\
\text{subject to} & |m| = M_\mathrm{s} \quad \text{on } \Omega\ , \\
& \mathrm{div}(\nabla u - \chi_\Omega m) = 0 \ \text{ in } \mathbb{R}^n\ , \\
& m\in L^\infty(\Omega;\mathbb{R}^n),\quad u\in W^{1,2}(\mathbb{R}^n),
\end{cases}
$$

i.e. minimization of anisotropy + exchange + magnetostatic + interaction energy;

$m:\Omega\to\mathbb{R}^n$= magnetization,

$u:\mathbb{R}^n\to\mathbb{R}$=magnetostatic potential,

∇u= demagnetizing field,

M_s= saturation magnetization (given).

Meso-scopical level (DeSimone (1993), Pedregal (1994)...):

zero-exchange energy limit: $\varepsilon \to 0$ and "$m_\varepsilon \overset{*}{\rightharpoonup} \nu$"

$$\begin{cases} \text{minimize} & E(\nu,u) - \displaystyle\int_\Omega h \cdot (\mathrm{id} \bullet \nu)\,\mathrm{d}x, \\ \text{where} & E(\nu,u) := \displaystyle\int_\Omega \varphi \bullet \nu \,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 \,\mathrm{d}x, \\ \text{subject to} & \mathrm{div}\Big(\nabla u - \chi_\Omega(\mathrm{id} \bullet \nu)\Big) = 0 \qquad \text{on } \mathbb{R}^3, \\ & \nu \in \mathcal{Y}(\Omega; S_{M_\mathrm{s}}), \qquad u \in W^{1,2}(\mathbb{R}^n), \end{cases}$$

where $\nu : \Omega \to \mathrm{rca}(S_{M_\mathrm{s}})$ is a Young measure,

thus $\nu_x \equiv \nu(x)$ describes volume fractions of m at x,

$[f \bullet \nu](x) := \int_{\mathbb{R}^3} f(m)\nu_x(\mathrm{d}m)$,

$\mathrm{id} : \mathbb{R}^3 \to \mathbb{R}^3$=the identity

then $\mathrm{id} \bullet \nu$=the macroscopical magnetization M,

$\mathcal{Y}(\Omega; S_{M_\mathrm{s}}) \subset L^\infty_\mathrm{w}(\Omega; \mathrm{rca}(S_{M_\mathrm{s}})) \cong L^1(\Omega; C(S_{M_\mathrm{s}}))^*$

the set of all Young measures,

S_{M_s}=the ball in $\mathbb{R}^n$ of the radius M_s.

A macro-scopical level (DeSimone (1993)):

$$\begin{cases} \text{minimize} & \displaystyle\int_\Omega \varphi_{\mathrm{eff}}(M) - h \cdot M \,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 \,\mathrm{d}x, \\ \text{subject to} & \mathrm{div}(\nabla u - \chi_\Omega M) = 0 \;\; \text{on } \mathbb{R}^3, \end{cases}$$

$\varphi_{\mathrm{eff}} := \big[\varphi + \delta_{S_{M_\mathrm{s}}}\big]^{**}$, M=macroscopical magnetization.

Evolution on the microscopical level:

Gilbert-Landau-Lifshitz model:

$$\frac{\partial m}{\partial t} = \lambda_1 m \times h_{\rm eff} - \lambda_2 m \times (m \times h_{\rm eff}),$$

$h_{\rm eff} := h - \varphi'(m) + \varepsilon\Delta m - \frac{1}{2}\nabla u$,

u again determined from $\mathrm{div}(\nabla u - \chi_\Omega m) = 0$,

φ'=the derivative of φ.

The balance of magnetic energy E_ε (test by $h_{\rm eff}$):

$$\frac{\mathrm{d}E_\varepsilon(m,u)}{\mathrm{d}t} = -\int_\Omega h_{\rm eff}\cdot\frac{\partial m}{\partial t}\,\mathrm{d}x = -\lambda_2\int_\Omega |m\times h_{\rm eff}|^2\mathrm{d}x \le 0,$$

which expresses Clausius-Duhem's inequality;

the “precession” λ_1-term does not dissipate energy,

the λ_2-term: a phenomenological “viscous” damping.

The multiwell structure of $\varphi|_{S_{M_{\rm s}}}$: a nearly rate-independent hysteretic response.

The width of the hysteresis loop in the m/h-diagram can thus be indirectly controlled by a shape of φ.

Evolution on the macroscopical level:

Rayleigh, Prandtl and Ishlinskiĭ model (1887) or Preisach's (1935) model (a continuum of activation thresholds)

Visintin (2000) (a one-threshold dry-friction)

Evolution on the mesoscopical level:

- rate-independent dissipation (independent of frequency of h)

Assumption: the amount of dissipated energy within the phase transformation from one pole to the other
= a single, phenomenologically given number (of the dimension J/m^3=Pa) depending on the coercive force H_c.

identification of poles through a vectorial *order parameter*:

$\mathcal{L} : S_{M_\mathrm{s}} \to \triangle_L$

$\triangle_L := \{\xi \in \mathbb{R}^L;\ \xi_i \geq 0,\ i = 1, ..., L,\ \sum_{i=1}^{L} \xi_i = 1\}.$

$\mathcal{L}_i(s)$ is equal 1 if s is in i-th pole, i.e. $s \in S_{M_\mathrm{s}}$ is in a neighborhood of i-th easy-magnetization direction.

$\lambda = \Lambda\nu := \mathcal{L} \bullet \nu$: mesoscopic order parameter

$[\mathcal{L} \bullet \nu](x) := \int_{S_{M_\mathrm{s}}} \mathcal{L}(s)\nu_x(\mathrm{d}s)$

$\varrho : \mathbb{R}^L \to \mathbb{R}_0^+$

$\varrho(\dot{\lambda}) = H_\mathrm{c}|\dot{\lambda}|_L$: specific dissipation potential

$|\cdot|_L$: a norm on $\mathbb{R}^L$

set of admissible configurations:

$$\mathcal{Q} : \ =\Big\{q = (\nu, \lambda) \in \mathcal{Y}(\Omega; S_{M_\mathrm{s}}) \times L^\infty(\Omega; \mathbb{R}^L)\ ;\quad \lambda(x) \in \triangle_L,\ \ \Lambda\nu = \lambda \text{ for a.a. } x \in \Omega\Big\}$$

Mielke's dissipation distance:

$$\delta(\lambda_1,\lambda_2) \quad := \quad \inf\Big\{ \int_0^1 \varrho(\frac{\mathrm{d}\lambda}{\mathrm{d}t})\,\mathrm{d}t; \quad \lambda\in C^1\big([0,1];\mathbb{R}^L\big), \\ \lambda(t)\in \mathrm{co}\mathcal{L}(S_{M_\mathrm{s}}),\ \lambda(0)=\lambda_1,\ \lambda(1)=\lambda_2 \Big\}.$$

in our case:

$$\delta(\lambda_1,\lambda_2) = H_\mathrm{c}|\lambda_1-\lambda_2|_L$$

total dissipation distance:

$$\mathcal{D}(q_1,q_2) := \int_\Omega \delta(\lambda_1,\lambda_2)\,\mathrm{d}x, \qquad q_i=(\nu_i,\lambda_i).$$

energy regularization (with $\alpha,\rho>0$):

$$\mathcal{E}_\rho(\nu,\lambda) := E(\nu) + \begin{cases} \rho||\lambda||^2_{W^{\alpha,2}(\Omega;\mathbb{R}^L)} & \text{if } \lambda\in W^{\alpha,2}(\Omega;\mathbb{R}^L), \\ +\infty & \text{otherwise,} \end{cases}$$

Zeeman's (external field) energy:

$$\langle H(t),q\rangle = \langle \nu, h(\cdot,t)\otimes \mathrm{id}\rangle;$$

Gibbs' energy:

$$\mathcal{G}(t,q) := \mathcal{E}_\rho(q) - \langle H(t),q\rangle$$

Mielke & Theil's definition of an *energetic solution*:

A process $q = q(t)$ is *stable* if $\forall t \in [0, T]$:

$$\forall \tilde{q} \in \mathcal{Q} : \qquad \mathcal{G}(t, q(t)) \leq \mathcal{G}(t, \tilde{q}) + \mathcal{D}(q(t), \tilde{q}).$$

A process $q = q(t)$ satisfies the *energy equality* if
$\forall t, s \in [0, T],\ s \leq t,$

$$\underbrace{\mathcal{G}(t, q(t))}_{\substack{\text{Gibbs' ener-}\\ \text{gy at time } t}} \; + \; \underbrace{\mathrm{Var}(\mathcal{D}, q; s, t)}_{\substack{\text{dissipated}\\ \text{energy}}}$$

$$= \; \underbrace{\mathcal{G}(s, q(s))}_{\substack{\text{Gibbs' ener-}\\ \text{gy at time } s}} \; - \underbrace{\int_s^t \Big\langle \frac{\mathrm{d}H}{\mathrm{d}t}, q(\theta) \Big\rangle \, \mathrm{d}\theta}_{\substack{\text{reduced work of}\\ \text{external field}}} \,,$$

$q = q(t) \equiv (\nu(t), \lambda(t))$ is an *energetic solution* if

- $\nu(t) \in \mathcal{Y}(\Omega; S_{M_{\mathrm{s}}})$ for all $t \in [0, T]$,
  $\lambda \in \mathrm{BV}([0, T]; L^1(\Omega; \mathbb{R}^L))$,
  $q(t) \in \mathcal{Q}$ for all $t \in [0, T]$,
- it is stable and satisfies the energy equality,
- $q(0) = q_0$.

The existence of an energetic solution:
a semi-discretization in time by the implicit Euler scheme with a time step $\tau > 0$, assuming T/τ an integer, and a sequence of τ's converging to zero, and such that, τ_i/τ_{i+1} is integer.

Then we put $q_\tau^0 = q_0$, a given initial condition, and, for $k = 1, ..., T/\tau$ we define q_τ^k recursively as a solution of the minimization problem

$$\left\{\begin{array}{ll} \text{Minimize} & I(q) := \mathcal{G}(k\tau, q) + \mathcal{D}(q_\tau^{k-1}, q) \\[1em] \text{subject to} & q \equiv (\nu, \lambda) \in \mathcal{Q} \ , \end{array}\right.$$

If a solution (i.e. a *global* minimizer) is not unique, we just take an arbitrary one for q_τ^k. Then we define the piecewise constant interpolation:

$$q_\tau(t) = \left\{\begin{array}{ll} q_\tau^k & \text{for } t \in ((k-1)\tau, k\tau], \\ q_0 & \text{for } t = 0. \end{array}\right.$$

A-priori estimates:

$$\begin{aligned} &\lambda_\tau \in L^\infty(0, T; H^\alpha(\Omega; \mathbb{R}^L) \cap L^\infty(\Omega; \mathbb{R}^L)) \\ &\qquad\quad \cap \mathrm{BV}([0, T]; L^1(\Omega; \mathbb{R}^L), \\ &\nu_\tau \in L^\infty(0, T; L^\infty_{\mathrm{w}}(\Omega; \mathrm{rca}(S_{M_\mathrm{s}})). \\ &\mathfrak{G}_\tau \in \mathrm{BV}([0, T]) \end{aligned}$$

where $\mathfrak{G}_\tau(t) := \mathcal{G}(t, q_\tau(t))$.

q_τ^k minimizes I & triangle inequality for $\mathcal{D}$

$$\Rightarrow \mathcal{G}(k\tau, q_\tau^k) \le \mathcal{G}(k\tau, \tilde{q}) + \mathcal{D}(q_\tau^{k-1}, \tilde{q}) - \mathcal{D}(q_\tau^{k-1}, q_\tau^k)$$
$$\le \mathcal{G}(k\tau, \tilde{q}) + \mathcal{D}(q_\tau^k, \tilde{q})$$

$\Rightarrow$ stability of q_τ:

$$\forall \tilde{q} \in \mathcal{Q} : \qquad \mathcal{G}(t, q_\tau(t)) \le \mathcal{G}(t, \tilde{q}) + \mathcal{D}(q_\tau(t), \tilde{q}).$$

1) stability of q_τ^{k-1} vs. $\tilde{q} := q_\tau^k$

2) q_τ^k minimizes I in comparison with q_τ^{k-1}

$\Rightarrow$ a two-sided energy inequality:

$$-\int_s^t \Big\langle \frac{\mathrm{d}H}{\mathrm{d}t}, q_\tau(\theta) \Big\rangle \mathrm{d}\theta$$
$$\le \mathcal{G}(t, q_\tau(t)) + \mathrm{Var}(\mathcal{D}, q_\tau; s, t) - \mathcal{G}(s, q_\tau(s))$$
$$\le -\int_s^t \Big\langle \frac{\mathrm{d}H}{\mathrm{d}t}, q_\tau(\theta - \tau) \Big\rangle \mathrm{d}\theta$$

Convergence for $\tau \to 0$ (Mielke-Francfort scheme):

Step 1a: Selection of a subsequence (Helly's theorem):

$\mathfrak{G} \in \mathrm{BV}([0,T]) : \quad \forall t \in [0,T] : \; \mathfrak{G}_\tau(t) \to \mathfrak{G}(t)$

$\lambda \in \mathrm{BV}([0,T]; L^1(\Omega; \mathbb{R}^L)) :$

$\qquad \forall t \in [0,T] : \; \lambda_\tau(t) \to \lambda(t)$ weakly in $L^1(\Omega; \mathbb{R}^L)$

$\mathfrak{P}_\tau := -\big\langle \frac{\mathrm{d}H}{\mathrm{d}t}, q_\tau \big\rangle \to \mathfrak{P}_*$ weakly in $L^1(0,T)$ and

$\mathfrak{P}(t) := \limsup_{\tau \to 0} \mathfrak{P}_\tau(t)$.

Step 1b: Selection of a finer net (Tikhonov theorem):

$\forall t \in [0,T] \quad \exists$ a Young measure $\nu(t) \in \mathcal{Y}(\Omega; S_{M_\mathrm{s}})$

$\exists \; \{q_{\tau_\xi}\}_{\xi \in \Xi}$ finer than the (sub)sequence $\{q_\tau\}$: $\;\nu_{\tau_\xi} \overset{*}{\rightharpoonup} \nu_t$

Step 2: Stability of the limit process q:
closedness of the graph of the stable-set mapping

$$t \mapsto \mathcal{S} := \big\{q \in \mathcal{Q} :\ \forall \tilde{q} \in \mathcal{Q} :\quad \mathcal{G}(t,q) \le \mathcal{G}(t,\tilde{q}) + \mathcal{D}(q,\tilde{q})\big\}.$$

Step 3: (Moore-Smith') convergence of the stored energy:
$\lim_{\xi\in\Xi} \mathcal{G}(t, q_{\tau_\xi}(t)) = \mathcal{G}(t, q(t))$ for any $t \in [0,T]$
so that $\mathfrak{G}_{\tau_\xi}(t) = \mathcal{G}(t, q(t))$

Step 4: Upper energy estimate:
limit passage in the 2$^{\rm nd}$ double-sided energy inequality

$$\Rightarrow \qquad \mathcal{G}(t,q(t)) + \mathrm{Var}(\mathcal{D},q;0,t) \le \mathcal{G}(0,q_0) + \int_0^t \mathfrak{P}_*(s)\mathrm{d}s$$

$$\le \mathcal{G}(0,q_0) + \int_0^t \mathfrak{P}(s)\,\mathrm{d}s$$

Step 5: Lower energy estimate:
a suitable partition $0 \le t_1^\varepsilon < t_2^\varepsilon < ...t_{k_\varepsilon}^\varepsilon \le T$,
stability of $q(t_{i-1}^\varepsilon)$ vs. $\tilde{q} := q(t_i^\varepsilon)$
approximation of a Lebesgue integral by Rieman's sums

$$\Rightarrow \qquad \mathcal{G}(t,q(t)) + \mathrm{Var}(\mathcal{D},q;0,t) \ge \mathcal{G}(0,q_0) + \int_0^t \mathfrak{P}(s)\,\mathrm{d}s. \qquad \Box$$

Remark:
1) $\mathfrak{P} = \mathfrak{P}_*$,
2) $t \mapsto \nu(t)$ weakly* measurable

$\Leftarrow$ a suitable a-posteriori selection
(A.Mainik, PhD-thesis 2004)

For uni-axial magnets (oriented in x_3-direction)

only the x_3-component of $\mathrm{id} \bullet \dot{\nu}$ dissipates:

the data φ and R can be considered, e.g., as

$$\varphi(m) = \varphi(m_1, m_2, m_3) = K(m_1^2 + m_2^2) \ ,$$
$$R(\dot{\nu}, \dot{u}) = \int_\Omega |\lambda \bullet \dot{\nu}| \, \mathrm{d}x \quad \text{with} \quad \lambda(m) = H_\mathrm{c} m_3;$$

K=the anisotropy parameter,

H_c=the coercive field

the point-wise explicit activation rule that triggers the magnetization evolution process:

$$\frac{\mathrm{d}M_3}{\mathrm{d}t}(x,t) \begin{cases} = 0 & \Longleftarrow \quad -H_\mathrm{c} < \mathfrak{H}(x,t) < H_\mathrm{c}, \\ > 0 & \Longrightarrow \quad \mathfrak{H}(x,t) = H_\mathrm{c}, \\ < 0 & \Longrightarrow \quad \mathfrak{H}(x,t) = -H_\mathrm{c}, \end{cases}$$

$\mathfrak{H} = \mathfrak{H}(x,t)$=an effective field;

$$\mathfrak{H}(x,t) \in H_c \mathrm{sign}(M_3(x,t)),$$

and $\nu_{x,t}$ must be supported only at those points s, $|s| = M_\mathrm{s}$, where the function

$$m \mapsto \varphi(m) + \mathfrak{H}(x,t) m_3 + (\nabla u(x,t) - h(x,t)) \cdot m$$

is minimized.

Numerical experiments:

x_3-axi-symmetrical geometry of Ω,

$h(x,t) = f(t)e_3$ spatially homogeneous, $e_3 = (0,0,1)$,

CoZrDy monocrystal at temperature $\theta = 4.2$ K,
easy-magnetization axis$=x_3$.

Anisotropy energy:

$$\varphi(m) = K\sin^2(\text{the angle between } m \text{ and } e_3),$$

$K = 40$ kJ/m^3, $M_\mathrm{s} = 0.05\,\mathrm{T}$, $H_\mathrm{c} = 20$ MA/m.

Various specimen shapes:

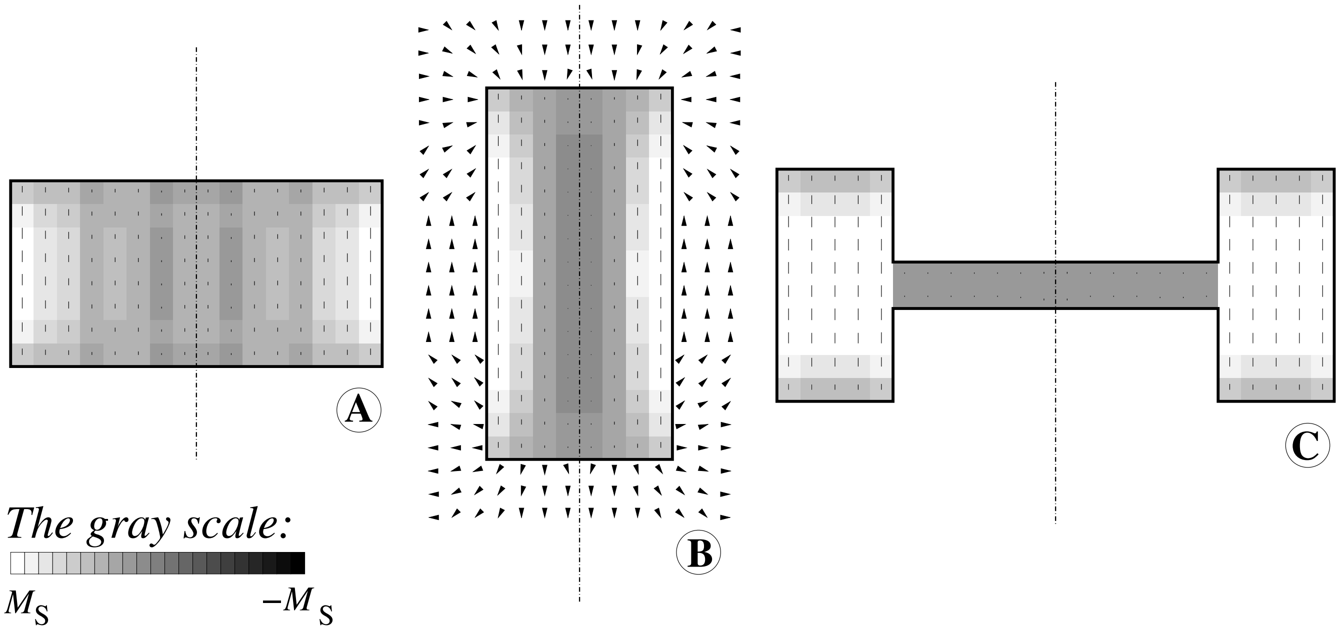

Fig.1: Cross-sections of various specimens with computed inhomogeneous magnetization (and for B also the demagnetizing field around) displayed at specific time instances.

The response depends on the shape:

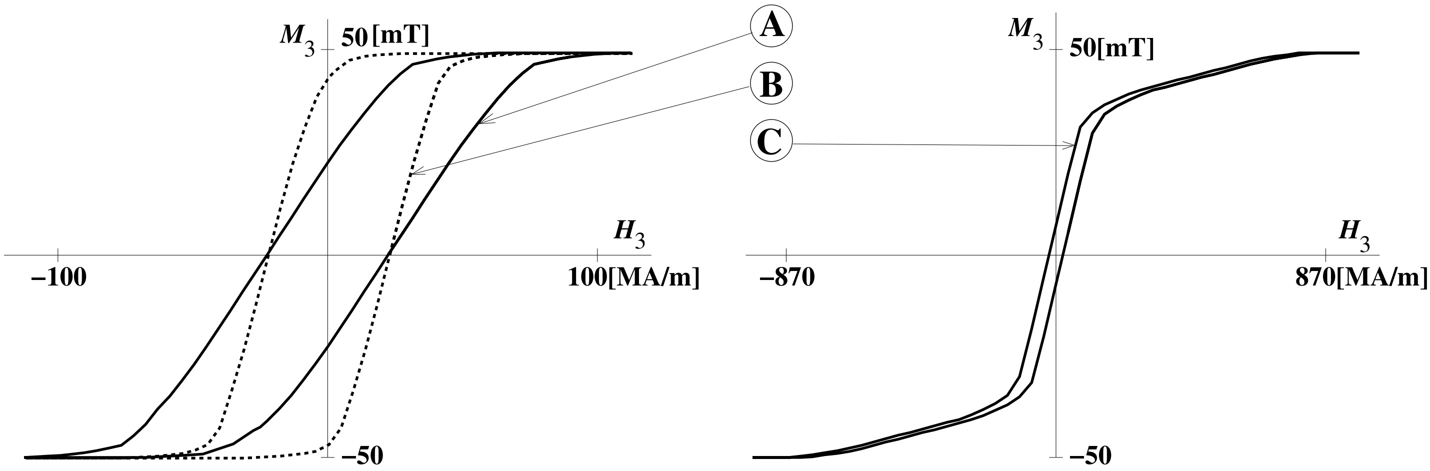

Fig.2: Corresponding hysteresis loops; the same material but different shapes of the specimen.

No minor loops observed $\Leftarrow$ only 1 activation threshold.

Spatial inhomogeneity of the coercive field $H_c = H_c(x)$: random variation $\pm 45\%$ around $H_c = 20$ MA/m: (two cases calculated)

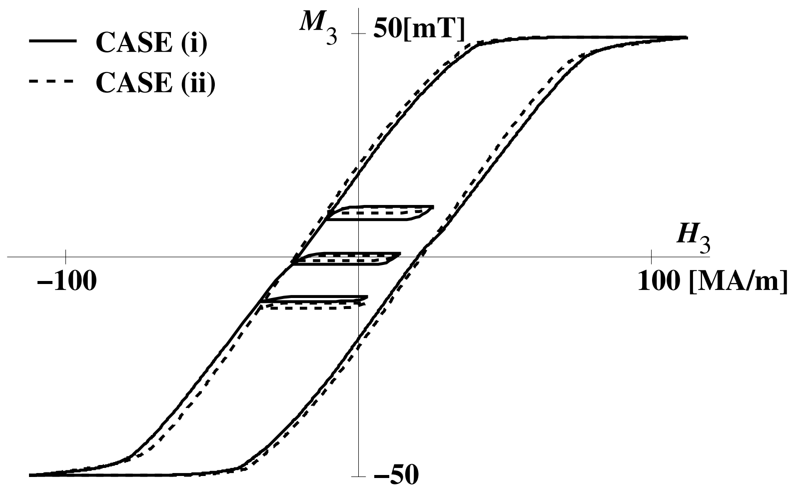

Fig.3: Minor hysteresis loops on the specimen A but with inhomogeneous material having randomly distributed coercive field $H_c = 20(\pm 45\%)$ MA/m.

The resulting macroscopical magnetization $M_3(x,t)$, t fixed, sometimes shows a tendency to self-organize by collective interactions to vertical stripes, which is obviously to minimize the energy of the created demagnetizing field.

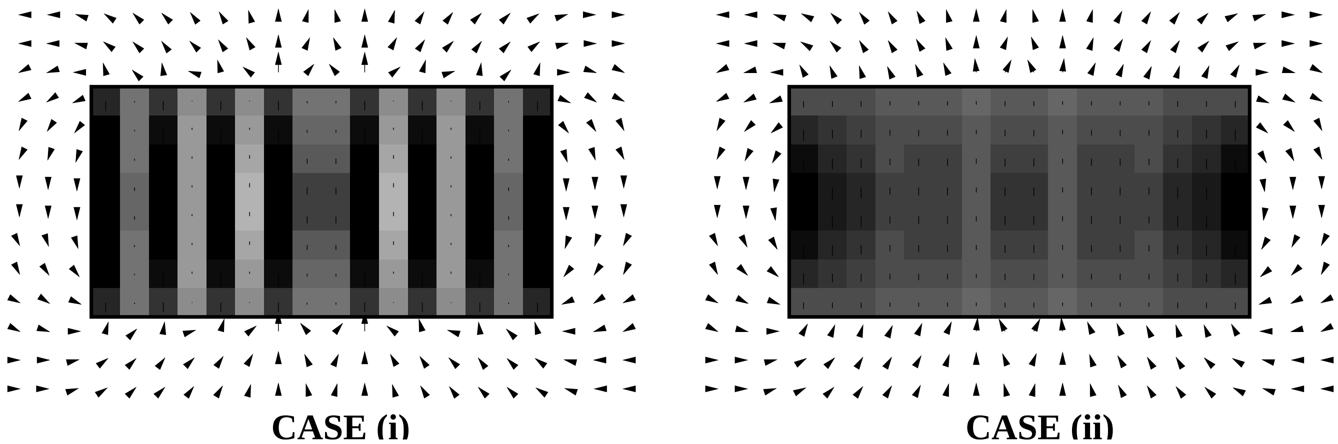

Fig.4: Computed magnetization on the specimen A with two cases of inhomogeneous material.

Virgin magnetization modeling: We make the coercive force depend on the history of the magnetization process, i.e., at the kth time step we consider

$$H_{\mathrm{c}}^{k-1}(x) := H_{\mathrm{c}}(x,(k-1)\tau) = \max_{0\le l\le k-1} \psi(M_3^l)$$

ψ a given positive continuous function e.g.

$$\psi(m_3) = \frac{H_{\mathrm{c,max}}}{1.3}\Big(\frac{|m_3|}{M_s} + 0.3\Big)$$

Then the energetic solution satisfying only upper energy estimate on $[0,t]$ can be proved to exist.

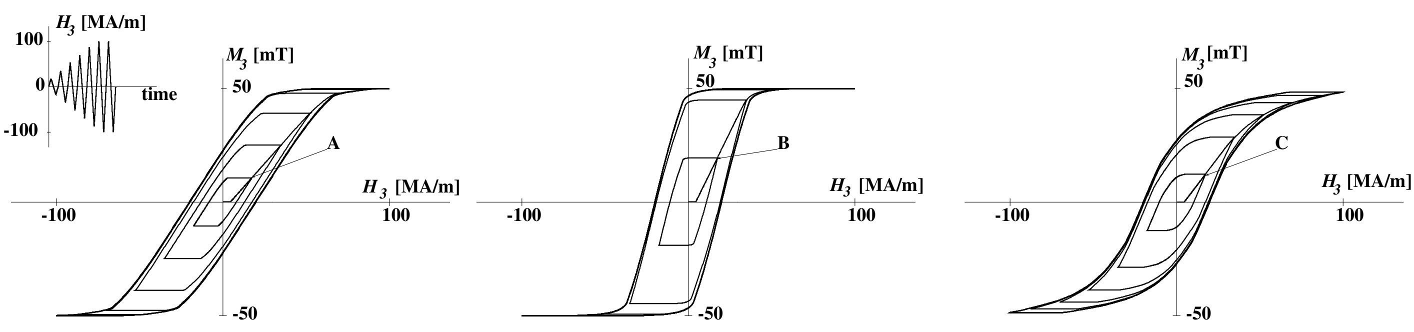

Fig.5: Minor-hysteresis-loop development as a response to an oscillating external field with an increasing amplitude. Various shapes of the magnet but the same material.

Thermodynamical evolution on mesoscopical level

M_s dependent on temperature θ,

ψ = specific Helmholtz free energy:

$$\psi(\nu,u,\theta)=\chi_\Omega\Big(\varphi\bullet\nu+\delta_{M_\mathrm{s}(\theta)}(\nu)-c\theta\ln(\theta)\Big)+\frac{1}{2}|\nabla u|^2,$$

$$\text{where }\delta_{M_\mathrm{s}(\theta)}(\nu):=\begin{cases}0 & \text{if supp}(\nu_x)\in S_{M_\mathrm{s}(\theta(x))}\\ & \qquad\qquad \text{for a.a. } x\in\Omega,\\ +\infty & \text{otherwise.}\end{cases}$$

c = specific heat

A temperature dependence of the dissipated energy (as well as of the anisotropy):

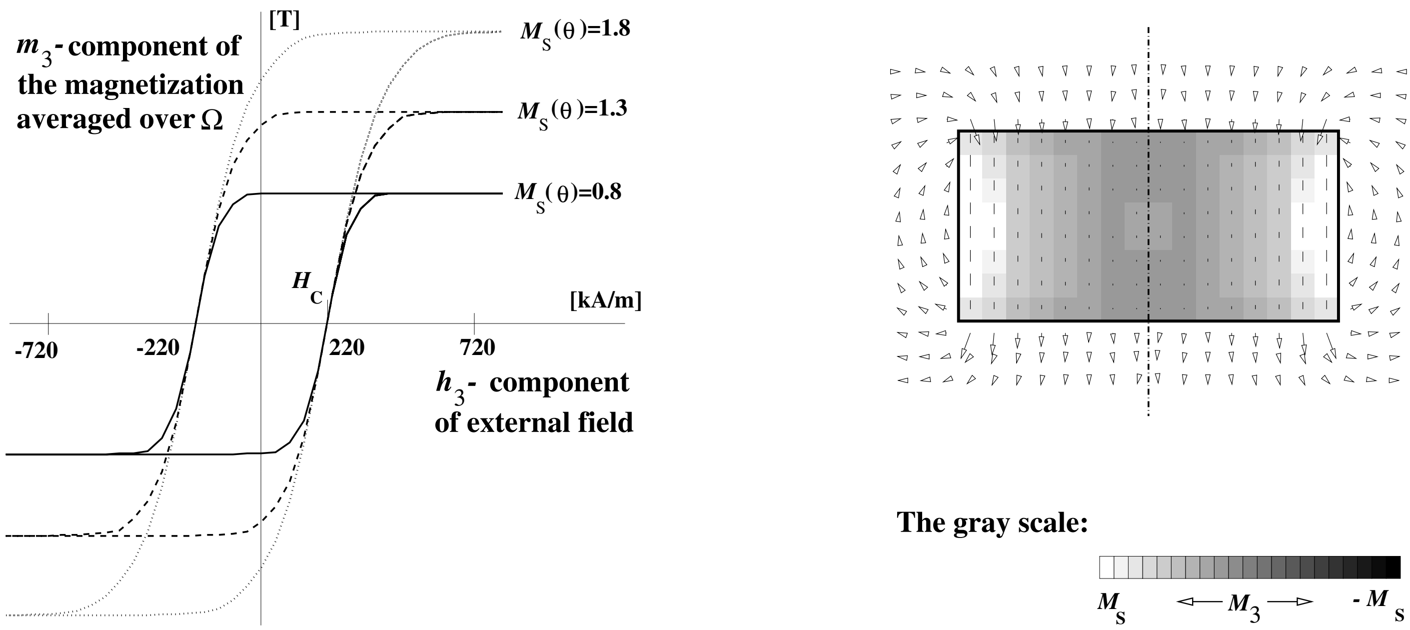

Fig.6: Dependence of h/m-hysteresis curves on H_s (left) calculated on a 2D specimen (right – and again one sample snapshot of the magnetization inside and demagnetizing field around Ω).

Normalized magnetization μ supported on the unit sphere $S_1 \subset \mathbb{R}^3$, i.e. $\mu \in \mathcal{Y}(\Omega; S_1)$, related with ν by

$$\nu = T^*_{M_s(\theta)}\mu, \qquad \text{with } \ T^*_{M_s(\theta)} = \big(T_{M_s(\theta)}\big)^*,$$
$$\text{where} \quad T_{M_s(\theta)}h(x,s) := h(x, M_s(\theta(x))s)$$

Special case: λ linear, φ quadratic:

the transformed specific free energy and dissipation rate:

$$\tilde\psi(\mu,u,\theta) = \chi_\Omega\left(M_s(\theta)^2\varphi\bullet\mu + \delta_1(\mu) - c\theta\ln(\theta)\right) + \frac12|\nabla u|^2,$$

$$\tilde\xi(\frac{d\mu}{dt},\theta) = M_s(\theta)\left|\lambda\bullet\frac{d\mu}{dt}\right|,$$

respectively. Now $u = u(\mu,\theta)$:

$$\operatorname{div}(\nabla u - M_s(\theta)\chi_\Omega(\mathrm{id}\bullet\mu)) = 0.$$

The transformed dynamics:

$$\partial_{(\mu,u)}\tilde R(\frac{d(\mu,u)}{dt},\theta) + \tilde\Psi'_{(\mu,u)}(\mu,u,\theta) + N_{\tilde Q(\theta)} \ni \tilde F(t,\theta)$$

with $\tilde\Psi(\mu,u,\theta) = \int_{\mathbb{R}^3}\tilde\psi(\mu,u,\theta)dx$,

$\tilde R(\frac{d}{dt}(\mu,u),\theta) = \tilde\xi(\frac{d}{dt}\mu,\theta)$

$\tilde Q(\theta) = \{(\mu,u)\in\mathcal{Y}(\Omega;S_1)\times W^{1,2}(\mathbb{R}^3);\ u = u(\mu,\theta)\}$,

$\tilde F(t,\theta) = (M_s(\theta)(h(t)\otimes\mathrm{id}),0)$.

The total free energy $\tilde\Psi(\mu,u,\theta) = \int_{\mathbb{R}^3}\tilde\psi(\mu,u,\theta)dx$.

The specific entropy s such that:

$$\int_{\mathbb{R}^3} sh\,dx = -\left[D_\theta\tilde\Psi(\mu,u,\theta)\right](h).$$

The nonlocal formula: $s = \chi_\Omega \Big(-2M_{\rm s}'(\theta)M_{\rm s}(\theta)(\varphi \bullet \mu)$

$- M_{\rm s}'(\theta)(\mathrm{id} \bullet \mu) \cdot \nabla\Delta^{-1}\mathrm{div}(\chi_\Omega M_{\rm s}(\theta)(\mathrm{id}\bullet\mu)) + c(1+\ln(\theta))\Big)$

Gibbs' relation $\Rightarrow$ the specific internal energy

$$e = \psi + \theta s = \chi_\Omega \Big((M_{\rm s}(\theta)^2 - 2\theta M_{\rm s}'(\theta)M_{\rm s}(\theta))(\varphi \bullet \mu)$$
$$- \theta M_{\rm s}'(\theta)(\mathrm{id}\bullet\mu)\cdot\nabla\Delta^{-1}\mathrm{div}(\chi_\Omega M_{\rm s}(\theta)(\mathrm{id}\bullet\mu)) + c\theta\Big) + \frac{1}{2}|\nabla u|^2.$$

The classical energy balance:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^3} e(x)\,\mathrm{d}x = \int_\Omega M_{\rm s}(\theta)h\cdot(\mathrm{id}\bullet\mu)\,\mathrm{d}x.$$

Altogether,

$$\int_\Omega \Big(\tilde\xi(\frac{\mathrm{d}\mu}{\mathrm{d}t}, \theta) - \theta\frac{\partial s}{\partial t}\Big)\,\mathrm{d}x = 0.$$

Fourier's law: the heat flux $=-\kappa\nabla\theta$

The entropy equation:

$$\theta\frac{\partial s}{\partial t} + \mathrm{div}(\kappa\nabla\theta) = \text{dissipation rate} = \tilde\xi(\frac{\mathrm{d}\mu}{\mathrm{d}t}, \theta)\ .$$

Substituting s gives the equation for temperature:

$$c\frac{\partial\theta}{\partial t} - \mathrm{div}(\kappa\nabla\theta) = M_{\rm s}(\theta)\left|\lambda\bullet\frac{\mathrm{d}\mu}{\mathrm{d}t}\right| - \theta\frac{\partial}{\partial t}\Big(2M_{\rm s}'(\theta)M_{\rm s}(\theta)(\varphi\bullet\mu)$$
$$+ M_{\rm s}'(\theta)(\mathrm{id}\bullet\mu)\cdot\nabla\Delta^{-1}\mathrm{div}(\chi_\Omega M_{\rm s}(\theta)(\mathrm{id}\bullet\mu))\Big).$$

Clausius-Duhem's inequality (with thermal isolation on $\partial\Omega$):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega s\,\mathrm{d}x = \int_\Omega \frac{\tilde{\xi}(\frac{\mathrm{d}\mu}{\mathrm{d}t},\theta) - \mathrm{div}(\kappa\nabla\theta)}{\theta}\,\mathrm{d}x$$
$$= \int_\Omega \frac{\tilde{\xi}(\frac{\mathrm{d}\mu}{\mathrm{d}t},\theta)}{\theta} + \kappa\frac{|\nabla\theta|^2}{\theta^2}\,\mathrm{d}x \geq 0\ .$$

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