

Modelling of Phase Transformations in magnetostrictive materials like NiMnGa

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reflecting collaboration with

GIUSEPPE TOMASSETTI

and

M.ARNDT, M.GRIEBEL, V.NOVÁK, P.PLECHÁČ, P.PODIO-GUIDUGLI,

K.R.RAJAGOPAL, P.ŠITTNER, C.ZANINI and others.

Content of the talk:

- 1 Phase transformations in NiMnGa
 - Martensitic/austenitic transformation
 - Ferro/para-magnetic transformation
 - Coupling of transformations: magnetostriction
- 2 The model and its analysis
 - Partly linearized ansatz
 - Analysis: semi-implicit discretisation, a-priori estimates
 - Analysis: convergence
- 3 Some other phenomena to be involved
 - General nonlinear ansatz
 - Pinning effects

Shape-memory materials (SMM): alloys (=SMAs) or intermetallics.

The mechanism behind **shape-memory effect** (=SME):

- o higher temperatures:

 - atoms tend to form a lattice with high symmetry (mostly cubic):

 - austenite** phase, higher heat capacity



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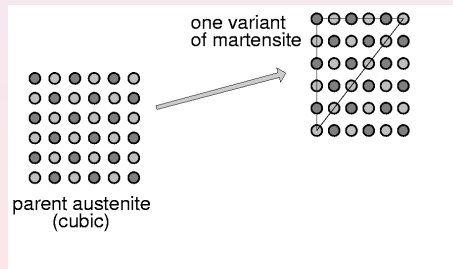
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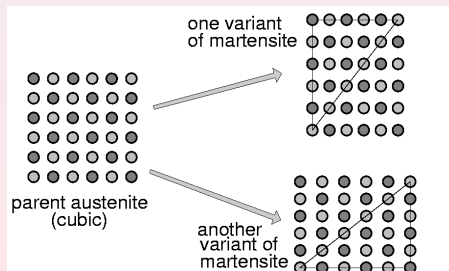
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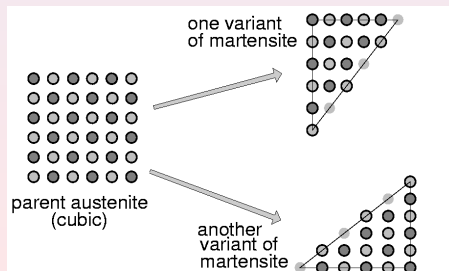
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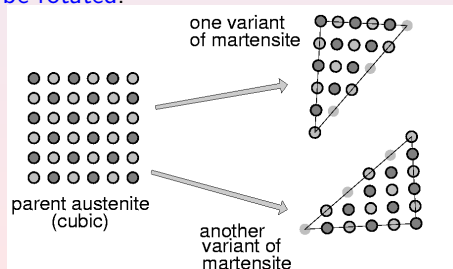
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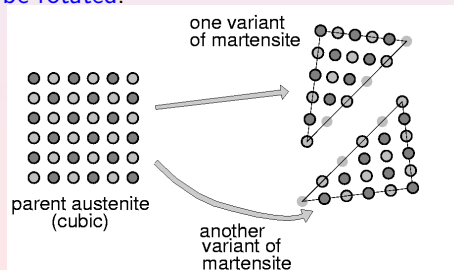
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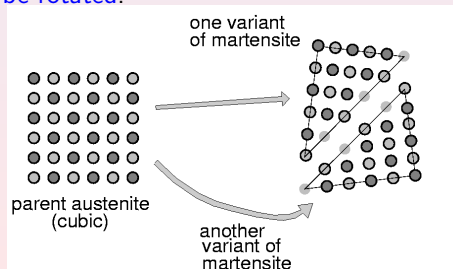
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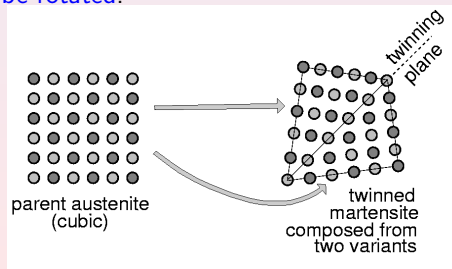
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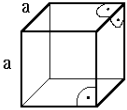
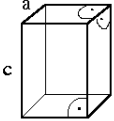
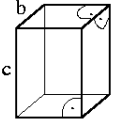
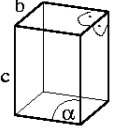
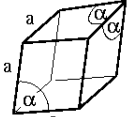
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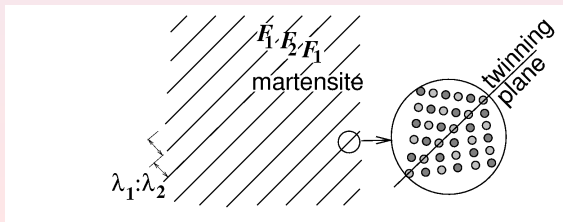
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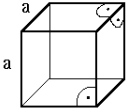
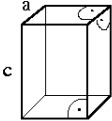
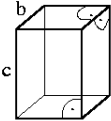
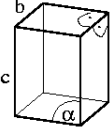
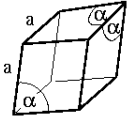
Crystallographical options of lower-symmetrical martensite:

				
cubic 1 variant	tetragonal 3 variants	orthorhombic 6 variants	monoclinic 12 variants	rhombic 4 variants
austenite	martensite in: NiMnGa, InTi		NiTi, CuZn	R-phase in NiTi

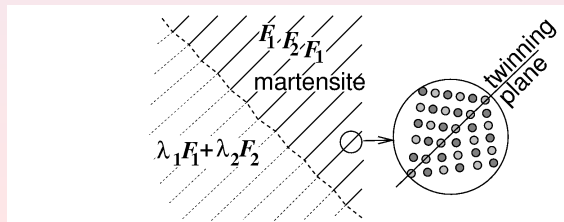
Self-accommodation of a microstructure in martensite



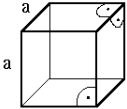
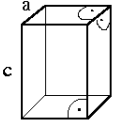
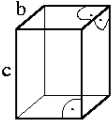
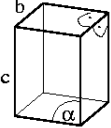
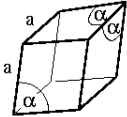
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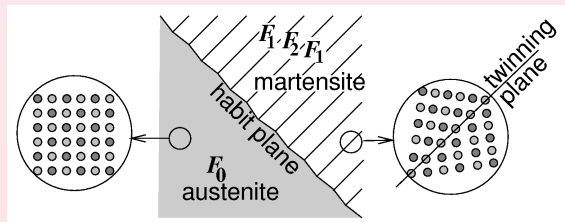
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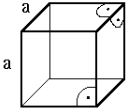
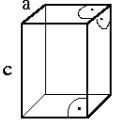
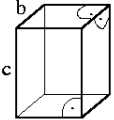
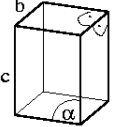
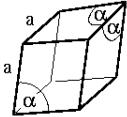
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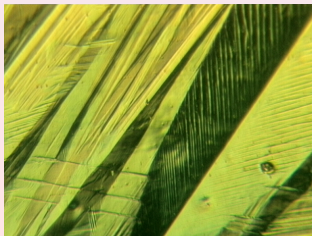
Self-accomodation of a microstructure in austenite and martensite



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1 variant	3 variants	6 variants	12 variants	4 variants
austenite	martensite in:			
	NiMnGa, InTi	CuAlNi, AuCd	NiTi, CuZn	R-phase in NiTi

Self-accomodation of a microstructure (example of CuAlNi)



Courtesy of

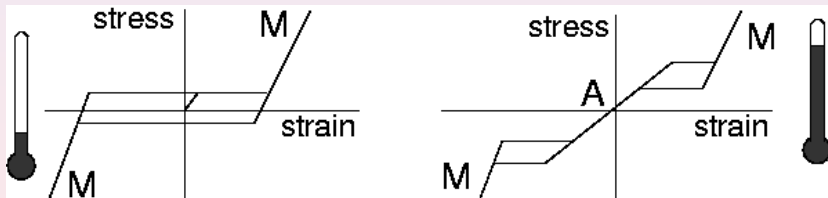
Václav Novák and Petr Šittner,
Institute of Physics,
Academy of Sciences, Czech Rep.

Schematic stress/strain response of SMM:

low temperature

vs

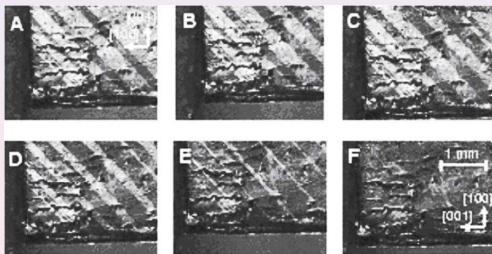
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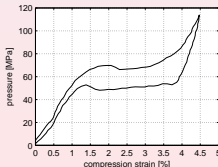
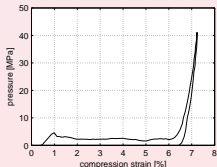
quasiplasticity

pseudoelasticity

Experiments by L.Straka, V.Novák, M.Landa, O.Heczko, 2004:
 Compression experiment: reorientation of tetragonal martensite in a
 (001)-oriented singlecrystal NiMnGa under temperature 293 K:

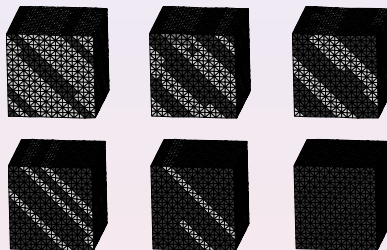


Stress-strain diagram at temperature 293 K (left) and 323 K (right):

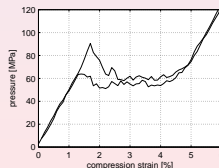
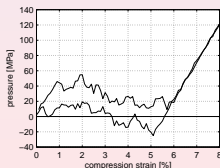


Computational simulations:

Compression experiment with NiMnGa (001)-oriented singlecrystal



Reorientation of martensite during a compression experiment at 293 K.



Stress/strain response during a compression experiment at 293 K and at 323 K.

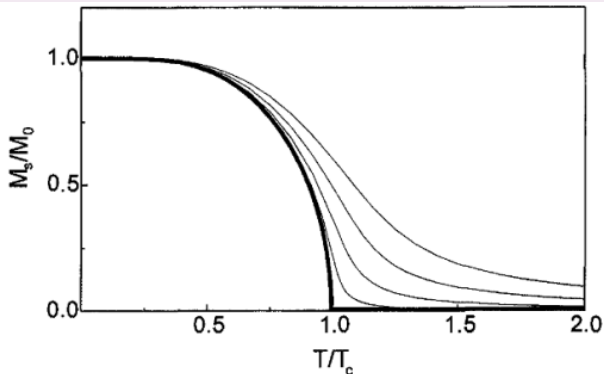
Calculations, visualizations: courtesy of Marcel Arndt, Universität Bonn.

Transformation in magnetic materials:

low temperature (below Currie point): highly-ordered, ferromagnetic state

very low temperature: the Heissenberg constraint $|m| = M_s$ is well satisfied
but in higher temperatures the deviation from it can be large in outer field

high temperature (above Currie point T_c): dis-ordered, paramagnetic state



FERRO-MAGNETIC



PARA-MAGNETIC

G.Bertotti: *Hysteresis in Magnetism*.

Academic Press, San Diego, 1998.

Both martensite/austenite and ferro/para-magnetic transformations are coupled:

Strong dependence of thermo-mechanical response on magnetic field in Ni₂MnGa single crystals – for example:

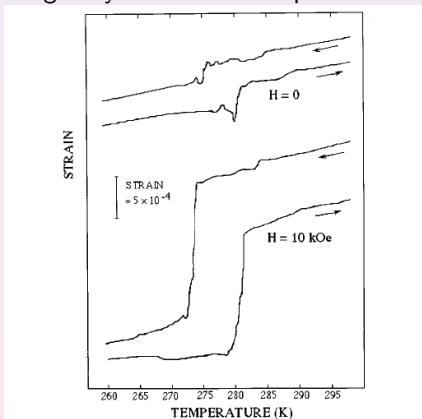


FIG. 2. Strain vs temperature in zero field and in 10 kOe. The two curves have been displaced relative to each other along the strain axis for clarity.

K.Ullakko, J.K.Huang, C.Kantner, R.C.O'Handley, V.V.Kokorin

in *Appl. Phys. Lett.* **69** (1996), 1966–1968.

Other phenomena to be captured:

electric resistivity depending on temperature and phase (an example in NiTi):

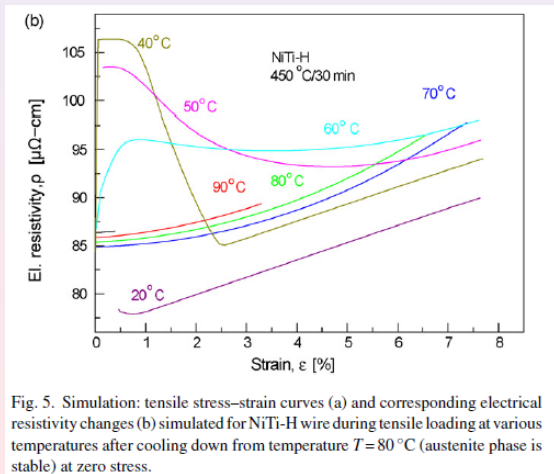


Fig. 5. Simulation: tensile stress-strain curves (a) and corresponding electrical resistivity changes (b) simulated for NiTi-H wire during tensile loading at various temperatures after cooling down from temperature $T=80^\circ\text{C}$ (austenite phase is stable) at zero stress.

V. Novák, P. Šittner, G.N. Dayananda, F.M. Braz-Fernandes, K.K. Mahesh,
Materials Science and Engineering A **481-482** (2008) 127-133

Variables (minimal scenario):

u displacement, $E(u) = \frac{1}{2}(\nabla u)^\top + \frac{1}{2}\nabla u =$ small-strain tensor,

m magnetisation,

θ temperature,

h magnetic field,

e electric field.

Basic concepts: small strains, Kelvin-Voigt rheology, 2nd-grade materials, electric displacement current (\sim electric-field energy) neglected,

\Rightarrow eddy-current approximation of the Maxwell equations,

partly linear free energy $\varphi(E, m, \theta) = \varphi_0(E, m) + \theta\varphi_1(E, m)$:

\Rightarrow heat capacity $c = -\varphi''_{\theta\theta} = -\varphi''_{\theta\theta}(\theta)$,

cross-effects neglected (no Peltier/Seebeck effects).

Main parameters of the model:

$\mathbb{K} = \mathbb{K}(E, m, \theta)$ thermal conductivity,

$\mathbb{S} = \mathbb{S}(E, m, \theta)$ electrical conductivity, $c = c(\theta)$ heat capacity,

$\gamma = \gamma(|m|)$ effective gyromagnetic ratio, μ_0 vacuum permeability,

α magnetic-dissipation constant, λ magnetic exchange-energy constant,

ρ mass density, f_0 bulk force (inertial and load),

\mathbb{D} viscosity tensor,

\mathbb{C}_H hyperelasticity tensor,

\mathbb{D}_H hyperviscosity tensor.

The equations:

Momentum equilibrium:

$$\rho \ddot{u} - \operatorname{div} \left(\varphi'_E(E(u), m, \theta) + \mathbb{D}E(\dot{u}) - \operatorname{div}(\mathbb{C}_H \nabla E(u) + \mathbb{D}_H \nabla E(\dot{u})) \right) = f_0 - \mu_0 \nabla h^\top m,$$

Landau-Lifshitz-Gilbert equation:

$$\alpha \dot{m} - \frac{m \times \dot{m}}{\gamma(|m|)} - \lambda \Delta m + \varphi'_m(E(u), m, \theta) = \mu_0 h,$$

heat equation

$$\begin{aligned} c(\theta) \dot{\theta} - \operatorname{div}(\mathbb{K}(E(u), m, \theta) \nabla \theta) &= \mathbb{S}(E(u), m, \theta) e : e + \mathbb{D}E(\dot{u}) : E(\dot{u}) + \mathbb{D}_H \nabla E(\dot{u}) : \nabla E(\dot{u}) \\ &+ \alpha |\dot{m}|^2 + \theta \varphi''_{E\theta}(E(u), m, \theta) : E(\dot{u}) + \theta \varphi''_{m\theta}(E(u), m, \theta) \cdot \dot{m}, \end{aligned}$$

Maxwell system (in eddy-current approximation):

$$\begin{aligned} \mu_0 (\dot{h} + \dot{m}) + \operatorname{curl} e &= -\mu_0 (\operatorname{div} \dot{u}) m - \mu_0 \nabla m \dot{u}, \\ \varepsilon_0 \dot{e} - \operatorname{curl} h + \mathbb{S}(E(u), m, \theta) e &= 0. \end{aligned}$$

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The equations: ...analysed for slow loading \Rightarrow pinning terms still needed

Momentum equilibrium:

K.R.RAJAGOPAL + T.R., 2003

$$\rho \ddot{u} - \operatorname{div} \left(\varphi'_E(E(u), m, \theta) + \mathbb{D}E(\dot{u}) - \operatorname{div}(\mathbb{C}_H \nabla E(u) + \mathbb{D}_H \nabla E(\dot{u})) \right) = f_0 - \mu_0 \nabla h^\top m,$$

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Derivation of the Maxwell system:

m_s = magnetisation in the physical space,
 “magnetic” part of the Maxwell system:

$$\mu_0(\dot{h} + \dot{m}_s) + \text{curl } e = 0$$

m = magnetisation in the reference configuration related with m_s by

$$\det(\mathbb{I} + \nabla u(t, x)) m_s(t, x + u(t, x)) = m(t, x).$$

Differentiation in time:

$$\det(\mathbb{I} + \nabla u) (\dot{m}_s + (\mathbb{I} + \nabla u)^{-\top} (\text{div } \dot{u}) m_s + \nabla m_s \dot{u}) = \dot{m}.$$

Small-displacement approximation $x + u \approx x$, which entails:

$\mathbb{I} + \nabla u \approx \mathbb{I}$, $m_s \approx m$, and $\nabla m_s \approx \nabla m$, so that

$$\dot{m}_s \approx \dot{m} - (\text{div } \dot{u}) m - \nabla m \dot{u} \quad \leftarrow \text{occurring as r.h.s. of the Maxwell system}$$

\dot{u} is not considered small

⇒ small but very fast mechanical vibrations

in some experiments on frequencies about 1 MHz or more.

Energetics:

Test: momentum eq. by \dot{u} , LLG by \dot{m} , heat eq. by 1, Maxwell by (h, e) :

Use: cancelation of the gyromagnetic term: $\frac{m \times \dot{m}}{\gamma(|m|)} \cdot \dot{m} = 0$,
 + cancelation of curl-terms + the identity:

$$\begin{aligned} \int_{\Omega} \underbrace{\mu_0((\operatorname{div} \dot{u})m + \nabla m \dot{u})}_{\text{r.h.s. of Maxwell eq.}} \cdot h \, dx &= \int_{\Omega} \mu_0 \operatorname{div}(m \otimes \dot{u}) \cdot h \, dx \\ &= \int_{\Omega} \mu_0 (\operatorname{div}((\dot{u} \otimes m)h) - (m \otimes \dot{u}) : \nabla h) \, dx \\ &= \int_{\Gamma} \mu_0 (m \cdot h)(\dot{u} \cdot n) \, dS - \int_{\Omega} \underbrace{\mu_0 \nabla h^T m \cdot \dot{u}}_{\text{r.h.s. of momentum equation}} \, dx \end{aligned}$$

$$\frac{d}{dt} \int_{\Omega} \underbrace{\varepsilon}_{\text{internal energy}} + \underbrace{\frac{\mu_0}{2}|h|^2}_{\text{magnetic energy}} + \underbrace{\frac{\rho}{2}|\dot{u}|^2}_{\text{kinetic energy}} \, dx = \int_{\Omega} \underbrace{f_0 \cdot \dot{u}}_{\text{power of external load}} \, dx + \text{boundary power.}$$

Gibbs' relation: $\psi = \varepsilon - s\theta$ with entropy $s = -\phi'_{\theta}$

internal energy: $\varepsilon = \vartheta + \psi(E, m, 0) + \frac{1}{2} C_H \nabla E : \nabla E + \frac{1}{2} \lambda |\nabla m|^2$, enthalpy $\vartheta = \int_{\theta}^{\theta} c(\cdot) \, d\theta$

Example of a free energy considered in NiMnGa:

described by the magnetization \mathbf{M} . A free-energy expansion is formulated in such a way that the functional is invariant under the actions \hat{O} of the space group of the fcc phase of Ni-Mn-Ga ($\hat{O}(F) \rightarrow F, \hat{O} \in O_h$), leading to

$$\begin{aligned}
 F = & \frac{1}{2}(c_{11} + 2c_{12})e_1^2 + \frac{1}{2}a(e_2^2 + e_3^2) + \frac{1}{2}c_{44}(e_4^2 + e_5^2 + e_6^2) + \frac{1}{3}be_3(e_3^2 - 3e_2^2) \\
 & + \frac{1}{4}c(e_2^2 + e_3^2)^2 + \frac{1}{\sqrt{3}}B_1e_1\mathbf{m}^2 + B_2 \left[\frac{1}{\sqrt{2}}e_2(m_x^2 - m_y^2) + \frac{1}{\sqrt{6}}e_3(3m_z^2 - \mathbf{m}^2) \right] \\
 & + B_3(e_4m_xm_y + e_5m_y m_z + e_6m_z m_x) + K_1(m_x^2m_y^2 + m_y^2m_z^2 + m_x^2m_z^2) \\
 & + \frac{1}{2}\alpha\mathbf{m}^2 + \frac{1}{4}\delta_1\mathbf{m}^4 - \mathbf{M}_0\mathbf{H}_0, \quad (1)
 \end{aligned}$$

where the e_i are linear combinations of the strain tensor components e_{ik} ,

$$\begin{aligned}
 e_1 &= (e_{xx} + e_{yy} + e_{zz})/\sqrt{3}, \\
 e_2 &= (e_{xx} - e_{yy})/\sqrt{2}, \\
 e_3 &= (2e_{zz} - e_{xx} - e_{yy})/\sqrt{6}, \\
 e_4 &= e_{xy}, e_5 = e_{yz}, e_6 = e_{zx}. \quad (2)
 \end{aligned}$$

In (1), a , b and c are linear combinations of the components of the second, third and fourth order elasticity moduli, respectively, with $a = c_{11} - c_{12}$, $b = (c_{111} - 3c_{112} + 2c_{123})/6\sqrt{6}$ and $c = (c_{1111} + 6c_{1112} - 3c_{1122} - 8c_{1123})/48$ (Fradkin, 1994); $\mathbf{m} = \mathbf{M}/M_0$ is the unit vector of the magnetization and M_0 saturation magnetization; B_i are magnetostriction constants; K_1 is the first cubic anisotropy constant; α_1 and δ_1 are exchange parameters.

in partly linearized ansatz:

critical points T_C and T_M the parameters a and α can be expressed as

$$a = a_0(T - T_M), \quad \alpha = \alpha_0(T - T_C),$$

A.T.Zayak, V.D.Buchelnikov, P.Entel: A Ginzburg-Landau theory for Ni-Mn-Ga.

Phase Trans. **75** (2002), 243-256

Fully implicit time-discretisation + regularization:

Recursive formula for the 5-tuple $(u_\tau^k, m_\tau^k, \vartheta_\tau^k, e_\tau^k, h_\tau^k)$ solving the system

Momentum-equilibrium equation:

$$\rho \frac{u_\tau^k - 2u_\tau^{k-1} + u_\tau^{k-2}}{\tau^2} - \operatorname{div} \left(S_\tau^k - \operatorname{div} H_\tau^k \right) = f_\tau^k - \mu_0 (\nabla h_\tau^k)^\top m_\tau^k \quad \text{with}$$

$$S_\tau^k := \sigma_E(E(u_\tau^k), m_\tau^k, \vartheta_\tau^k) + \mathbb{D}E\left(\frac{u_\tau^k - u_\tau^{k-1}}{\tau}\right) + \tau |E(u_\tau^k)|^{\eta-2} E(u_\tau^k), \quad \text{and}$$

$$H_\tau^k := \mathbb{D}_H \nabla E\left(\frac{u_\tau^k - u_\tau^{k-1}}{\tau}\right) + C_H \nabla E(u_\tau^k) + \tau |\nabla E(u_\tau^k)|^{\eta-2} \nabla E(u_\tau^k),$$

Landau-Lifshitz-Gilbert equation:

$$\alpha \frac{m_\tau^k - m_\tau^{k-1}}{\tau} - \frac{m_\tau^k}{\gamma(|m_\tau^k|)} \times \frac{m_\tau^k - m_\tau^{k-1}}{\tau} - \lambda \Delta m_\tau^k + \sigma_m(E(u_\tau^k), m_\tau^k, \vartheta_\tau^k)$$

$$- \mu_0 h_\tau^k = \tau \operatorname{div}(|\nabla m_\tau^k|^{\eta-2}) \nabla m_\tau^k - \tau |m_\tau^k|^{\eta-2} m_\tau^k,$$

Heat equation:

$$\begin{aligned} \frac{\vartheta_\tau^k - \vartheta_\tau^{k-1}}{\tau} - \operatorname{div} \left(K_0(E_\tau^k, m_\tau^k, \vartheta_\tau^k) \nabla \vartheta_\tau^k \right) &= S(E_\tau^k, m_\tau^k, \vartheta_\tau^k) e_\tau^k : e_\tau^k \\ &+ \left(1 - \frac{\sqrt{\tau}}{2} \right) \mathbb{D} E \left(\frac{u_\tau^k - u_\tau^{k-1}}{\tau} \right) : E \left(\frac{u_\tau^k - u_\tau^{k-1}}{\tau} \right) \\ &+ \mathbb{D}_H \nabla E \left(\frac{u_\tau^k - u_\tau^{k-1}}{\tau} \right) : \nabla E \left(\frac{u_\tau^k - u_\tau^{k-1}}{\tau} \right) \\ &+ \left(1 - \frac{\sqrt{\tau}}{2} \right) \alpha \left| \frac{m_\tau^k - m_\tau^{k-1}}{\tau} \right|^2 + A \left(E_\tau^k, m_\tau^k, \vartheta_\tau^k; \frac{E_\tau^k - E_\tau^{k-1}}{\tau}, \frac{m_\tau^k - m_\tau^{k-1}}{\tau} \right), \end{aligned}$$

Maxwell system:

$$\begin{aligned} \frac{h_\tau^k - h_\tau^{k-1}}{\tau} + \frac{\operatorname{curl} e_\tau^k}{\mu_0} &= \nabla m_\tau^k \frac{u_\tau^k - u_\tau^{k-1}}{\tau} - \frac{m_\tau^k - m_\tau^{k-1}}{\tau} + \operatorname{div} \frac{u_\tau^k - u_\tau^{k-1}}{\tau} m_\tau^k, \\ \operatorname{curl} h_\tau^k - S(E_\tau^k, m_\tau^k, \vartheta_\tau^k) e_\tau^k &= \tau |e_\tau^k|^{\eta-2} e_\tau^k, \end{aligned}$$

for $k = 1, \dots, K_\tau := T/\tau$, where we abbreviated $E_\tau^k = E(u_\tau^k)$ and

$$A(E, m, \vartheta; \dot{E}, \dot{m}) = \theta \varphi''_{E\theta}(E, m, \theta) : \dot{E} + \theta \varphi''_{m\theta}(E, m, \theta) \cdot \dot{m}$$

$$\text{with } \theta = \widehat{c}^{-1}(\vartheta) \text{ and } \widehat{c}' = c_{\dots}$$

We use the discrete scheme recursively, starting from $k = 1$ by using

$$u_\tau^0 = u_{0,\tau}, \quad u_\tau^{-1} = u_{0,\tau} - \tau v_0, \quad m_\tau^0 = m_{0,\tau}, \quad \vartheta_\tau^0 = \hat{c}(\theta_0), \quad h_\tau^0 = h_0,$$

Existence of $(u_\tau^k, m_\tau^k, \vartheta_\tau^k, e_\tau^k, h_\tau^k)$:

η large enough (namely $\eta > 8$) \Rightarrow pseudomonotone coercive operator
 \Rightarrow Brézis' theorem \Rightarrow

$$u_\tau^k \in W^{2,\eta}(\Omega; \mathbb{R}^3),$$

$$m_\tau^k \in W^{1,\eta}(\Omega; \mathbb{R}^3),$$

$$\vartheta_\tau^k \in W^{1,2}(\Omega),$$

$$h_\tau^k \in L_{\text{curl}}^{2,\eta'}(\Omega; \mathbb{R}^3),$$

$$e_\tau^k \in L_{\text{curl}}^{\eta,2}(\Omega; \mathbb{R}^3)$$

where $L_{\text{curl}}^{p,q}(\Omega; \mathbb{R}^3) := \{v \in L^p(\Omega; \mathbb{R}^3); \text{curl } v \in L^q(\Omega; \mathbb{R}^3)\}$.

Non-negativity: $\vartheta_\tau^k \geq 0$.

A-priori estimates (u_τ, \bar{u}_τ etc. are interpolants over $[0, T]$):

Energy-type test (by $\dot{u}_\tau, \dot{m}_\tau, 1, \bar{h}_\tau, \bar{e}_\tau$) \Rightarrow

$$\|u_\tau\|_{W^{1,\infty}(I;L^2(\Omega;\mathbb{R}^3))\cap W^{1,2}(I;W^{2,2}(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|m_\tau\|_{L^\infty(I;W^{1,2}(\Omega;\mathbb{R}^3))\cap W^{1,2}(I;L^2(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|\bar{v}_\tau\|_{L^\infty(I;L^1(\Omega))} \leq C,$$

$$\|h_\tau\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|\bar{e}_\tau\|_{L^2(Q;\mathbb{R}^3)} \leq C,$$

$$\|E(\bar{u}_\tau)\|_{L^\infty(I;W^{1,\eta}(\Omega;))} \leq C\tau^{-1/\eta},$$

$$\|m_\tau\|_{L^\infty(I;W^{1,\eta}(\Omega;\mathbb{R}^3))} \leq C\tau^{-1/\eta},$$

$$\|e_\tau\|_{L^\eta(Q;\mathbb{R}^3)} \leq C\tau^{-1/\eta}$$

based on the semi-convexity of the functional (for enough small $\tau > 0$)

$$(E, m) \mapsto \varphi(E, m) + \frac{\tau}{\eta}|E|^\eta + \frac{\tau}{\eta}|m|^\eta + \frac{\mathbb{D}E:E + \alpha|m|^2}{2\sqrt{\tau}}$$

A-priori estimates (u_τ, \bar{u}_τ etc. are interpolants over $[0, T]$):

Energy-type test (by $\dot{u}_\tau, \dot{m}_\tau, 1, \bar{h}_\tau, \bar{e}_\tau$) \Rightarrow

$$\|u_\tau\|_{W^{1,\infty}(I;L^2(\Omega;\mathbb{R}^3)) \cap W^{1,2}(I;W^{2,2}(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|m_\tau\|_{L^\infty(I;W^{1,2}(\Omega;\mathbb{R}^3)) \cap W^{1,2}(I;L^2(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|\bar{v}_\tau\|_{L^\infty(I;L^1(\Omega))} \leq C,$$

$$\|h_\tau\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|\bar{e}_\tau\|_{L^2(Q;\mathbb{R}^3)} \leq C,$$

$$\|E(\bar{u}_\tau)\|_{L^\infty(I;W^{1,\eta}(\Omega;))} \leq C\tau^{-1/\eta},$$

$$\|m_\tau\|_{L^\infty(I;W^{1,\eta}(\Omega;\mathbb{R}^3))} \leq C\tau^{-1/\eta},$$

$$\|e_\tau\|_{L^\eta(Q;\mathbb{R}^3)} \leq C\tau^{-1/\eta}$$

based on the semi-convexity of the functional (for enough small $\tau > 0$)

$$(E, m) \mapsto \varphi(E, m) + \frac{\tau}{\eta}|E|^\eta + \frac{\tau}{\eta}|m|^\eta + \frac{\mathbb{D}E:E + \alpha|m|^2}{2\sqrt{\tau}}$$

A-priori estimates (u_τ, \bar{u}_τ etc. are interpolants over $[0, T]$):

Energy-type test (by $\dot{u}_\tau, \dot{m}_\tau, 1, \bar{h}_\tau, \bar{e}_\tau$) \Rightarrow

$$\|u_\tau\|_{W^{1,\infty}(I;L^2(\Omega;\mathbb{R}^3))\cap W^{1,2}(I;W^{2,2}(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|m_\tau\|_{L^\infty(I;W^{1,2}(\Omega;\mathbb{R}^3))\cap W^{1,2}(I;L^2(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|\bar{\vartheta}_\tau\|_{L^\infty(I;L^1(\Omega))} \leq C,$$

$$\|h_\tau\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \leq C,$$

$$\|\bar{e}_\tau\|_{L^2(Q;\mathbb{R}^3)} \leq C,$$

$$\|E(\bar{u}_\tau)\|_{L^\infty(I;W^{1,\eta}(\Omega;))} \leq C\tau^{-1/\eta},$$

$$\|m_\tau\|_{L^\infty(I;W^{1,\eta}(\Omega;\mathbb{R}^3))} \leq C\tau^{-1/\eta},$$

$$\|e_\tau\|_{L^\eta(Q;\mathbb{R}^3)} \leq C\tau^{-1/\eta},$$

+ a special nonlinear test of the heat equation + Gagliardo-Nirenberg interpolation

$$\|\nabla\bar{\vartheta}_\tau\|_{L^r(Q;\mathbb{R}^d)} \leq C_r \quad \text{with } r < 5/4.$$

Further a-priori estimates:

$$\left\| \varrho \ddot{u}_\tau^i \right\|_{L^2(I; W^{2,2}(\Omega; \mathbb{R}^3)^*) + L^{\eta'}(I; W^{2,\eta}(\Omega; \mathbb{R}^3)^*)} \leq C,$$

$$\left\| \varrho \ddot{u}_\tau^i - \tau \operatorname{div}(|E(\bar{u}_\tau)|^{\eta-2} E(\bar{u}_\tau)) + \tau \operatorname{div}^2(|\nabla E(\bar{u}_\tau)|^{\eta-2} \nabla E(\bar{u}_\tau)) \right\|_{L^2(I; W^{2,2}(\Omega; \mathbb{R}^3)^*)} \leq C,$$

$$\left\| \dot{\vartheta}_\tau \right\|_{L^1(I; W^{3,2}(\Omega)^*)} \leq C,$$

$$\left\| \operatorname{curl} \bar{h}_\tau + \tau |\bar{e}_\tau|^{\eta-2} \bar{e}_\tau \right\|_{L^2(Q; \mathbb{R}^3)} \leq C,$$

$$\left\| \dot{h}_\tau \right\|_{L^2(I; L^2_{\operatorname{curl},0}(\Omega; \mathbb{R}^3)^*)} \leq C.$$

Convergence for $\tau \rightarrow 0$: Step 0: Banach' selection principle:

$$\begin{array}{ll}
 u_\tau \rightarrow u & \text{strongly in } W^{1,2}(I; W^{2,2}(\Omega; \mathbb{R}^3)), \\
 m_\tau \rightarrow m & \text{strongly in } W^{1,2}(I; W^{1,2}(\Omega; \mathbb{R}^3)), \\
 \vartheta_\tau \rightarrow \vartheta & \text{strongly in } L^s(Q) \text{ with any } s < 5/3, \\
 \bar{e}_\tau \rightarrow e & \text{strongly in } L^2(Q; \mathbb{R}^3), \\
 \bar{h}_\tau \rightarrow h & \text{weakly* in } L^\infty(I; L^2(\Omega; \mathbb{R}^3)),
 \end{array}$$

and, moreover (with h_b from not-mentioned boundary conditions)

$$\begin{array}{ll}
 \bar{h}_\tau - \bar{h}_{b,\tau} \rightarrow h - h_b & \text{weakly in } L^{\eta'}(I; L^2_{\text{curl},0}{}^{\eta'}(\Omega; \mathbb{R}^3)), \text{ and} \\
 \text{curl } \bar{h}_\tau + \tau |\bar{e}_\tau|^{\gamma-2} \bar{e}_\tau \rightarrow \text{curl } h & \text{weakly in } L^2(Q; \mathbb{R}^{3 \times 3}).
 \end{array}$$

for a subsequence.

Then we want to prove that any (u, m, ϑ, h, e) obtained in this way is a weak solution to the considered IBVP (after the transformation $\theta \mapsto \vartheta$) which also preserves the total energy.

Step 1: Convergence in the semilinear mechanical/magnetic/electro part:

Aubin-Lions' theorem: strong convergence of $E(\bar{u}_\tau)$, \bar{m}_τ , and \bar{v}_τ .

Then weak convergence suffices in semilinear terms, while the quasilinear regularizing terms vanish, e.g.

$$\left| \int_Q \tau |E(\bar{u}_\tau)|^{\eta-2} E(\bar{u}_\tau) : E(v) \, dx dt \right| \leq \tau \|E(\bar{u}_\tau)\|_{L^\eta(Q; \mathbb{R}^{3 \times 3})}^{\eta-1} \|E(v)\|_{L^\eta(Q; \mathbb{R}^{3 \times 3})}$$

$$\leq C \tau^{1/\eta} \|E(v)\|_{L^\eta(Q; \mathbb{R}^{3 \times 3})} \rightarrow 0$$

for any smooth v .

Step 2: Mechanical/magnetic energy preservation:

test respectively by \dot{u} , \dot{m} , h , and e and make the by-part integration

$$\rho \ddot{u}_\tau^i - \tau \operatorname{div}(|E(\bar{u}_\tau)|^{\eta-2} E(\bar{u}_\tau)) + \tau \operatorname{div}^2(|\nabla E(\bar{u}_\tau)|^{\eta-2} \nabla E(\bar{u}_\tau)) \rightharpoonup \zeta \in L^2(I; W^{2,2}(\Omega; \mathbb{R}^3)^*)$$

and then

$$\langle \zeta, w \rangle = \lim_{\tau \rightarrow 0} \int_Q \rho \dot{u}_\tau^i \cdot \dot{w} - \tau |E(\bar{u}_\tau)|^{\eta-2} E(\bar{u}_\tau) : E(w) + \tau |\nabla E(\bar{u}_\tau)|^{\eta-2} \nabla E(\bar{u}_\tau) : \nabla E(w) \, dx dt = \int_Q \rho \dot{u} \cdot \dot{w} \, dx dt.$$

$$\Rightarrow \zeta = \rho \ddot{u} \Rightarrow \rho \ddot{u} \text{ is in duality with } \dot{u} \in L^2(I; W^{2,2}(\Omega; \mathbb{R}^3)).$$

Step 3: Strong convergence of $\nabla E(\dot{u}_\tau)$ and \dot{m}_τ and \bar{e}_τ :

$$\begin{aligned}
 & \int_Q \mathbb{D}E(\dot{u}):E(\dot{u}) + \mathbb{D}_H \nabla E(\dot{u}):\nabla E(\dot{u}) + \alpha|\dot{m}|^2 + S(E, m, \vartheta)e \cdot e \\
 & \leq \liminf_{\tau \rightarrow 0} \int_Q \mathbb{D}E(\dot{u}_\tau):E(\dot{u}_\tau) + \mathbb{D}_H \nabla E(\dot{u}_\tau):\nabla E(\dot{u}_\tau) + \alpha|\dot{m}_\tau|^2 + S(\bar{E}_\tau, \bar{m}_\tau, \bar{\vartheta}_\tau)\bar{e}_\tau \cdot \bar{e}_\tau dx \\
 & \leq \limsup_{\tau \rightarrow 0} \int_Q \mathbb{D}E(\dot{u}_\tau):E(\dot{u}_\tau) + \mathbb{D}_H \nabla E(\dot{u}_\tau):\nabla E(\dot{u}_\tau) + \alpha|\dot{m}_\tau|^2 + S(\bar{E}_\tau, \bar{m}_\tau, \bar{\vartheta}_\tau)\bar{e}_\tau \cdot \bar{e}_\tau dx \\
 & \leq \limsup_{\tau \rightarrow 0} \Phi(u_{0\tau}, v_0, m_{0\tau}, h_0) - \Phi(u_\tau(T), \dot{u}_\tau(T), m_\tau(T), h_\tau(T)) \\
 & + \int_\Omega \frac{\tau}{\eta} |E(u_{0\tau})|^\eta + \frac{\tau}{\eta} |\nabla E(u_{0\tau})|^\eta + \frac{\tau}{\eta} |m_{0\tau}|^\eta dx - \int_\Sigma \bar{g}_\tau \cdot \dot{u}_\tau dt + \int_Q \bar{f}_\tau \cdot \dot{u}_\tau + \text{curl } h_{b,\tau} \cdot e_\tau \\
 & \quad + \mu_0 (\dot{h}_\tau + \dot{m}_\tau - \nabla \bar{m}_\tau \dot{u}_\tau - (\text{div } \dot{u}_\tau)_\tau) \cdot h_{b,\tau} - A(\bar{E}_\tau, \bar{m}_\tau, \bar{\vartheta}_\tau; \dot{E}_\tau, \dot{m}_\tau) dx dt \\
 & \leq \Phi(u_0, v_0, m_0, h_0) - \Phi(u(T), \dot{u}(T), m(T), h(T)) - \int_\Sigma g \cdot \dot{u} dt + \int_Q f \cdot \dot{u} + \text{curl } h_b \cdot e \\
 & \quad + \mu_0 (\dot{h} + \dot{m} - \nabla m \dot{u} - (\text{div } \dot{u})m) \cdot h_b - A(E, m, \vartheta; \dot{E}, \dot{m}) dx dt \\
 & = \int_Q \mathbb{D}E(\dot{u}):E(\dot{u}) + \mathbb{D}_H \nabla E(\dot{u}):\nabla E(\dot{u}) + \alpha|\dot{m}|^2 + S(E, m, \vartheta)e \cdot e.
 \end{aligned}$$

Step 4: Limit passage in the heat equation:

Having proved the strong convergence in Step 2, the right-hand side of the heat equation converges strongly in $L^1(Q)$ and this limit passage is then easy.

Step 5: Total energy preservation:

We have $\dot{\vartheta} \in L^1(I; W^{3,2}(\Omega)^*)$, and realize the already proved the heat equation, which is in duality with the constant 1, we can perform rigorously this test and sum it with mechanical/magnetic energy balance obtained already in Step 2.

Fully nonlinear coupling:

more symmetry \sim higher heat capacity

heat capacity is higher in austenite than in martensite

\Rightarrow shape-memory effect

c should depend rather directly on E (and also m , not only on θ)

fully **general nonlinear ansatz** $\varphi(E, m, \theta)$ instead of $\varphi_0(E, m) + \theta\varphi_1(E, m)$

then the **heat capacity** $c = -\psi''_{\theta\theta}$ depends, beside θ , also on E and m .

Generalized enthalpy transformation:

$$\vartheta = \hat{c}(E, m, \theta) := \int_0^\theta c(E, m, \Theta) d\Theta$$

$$c(E, m, \theta)\dot{\theta} = \frac{\partial \hat{c}(E, m, \theta)}{\partial t} - c_1(E, m, \theta):\dot{E} - c_2(E, m, \theta)\cdot\dot{m},$$

$$c_1(E, m, \theta) = \int_0^\theta c'_E(E, m, \Theta) d\Theta \quad \text{and} \quad c_2(E, m, \theta) = \int_0^\theta c'_m(E, m, \Theta) d\Theta.$$

Define: $\mathcal{T}(E, m, \cdot) := [\hat{c}(E, m, \cdot)]^{-1}$

$$\mathcal{K}_0(E, m, \vartheta) := \mathbb{K}(E, m, \mathcal{T}(E, m, \vartheta))\mathcal{T}'_{\vartheta}(E, m, \vartheta),$$

$$\mathcal{K}_1(E, m, \vartheta) := \mathbb{K}(E, m, \mathcal{T}(E, m, \vartheta))\mathcal{T}'_E(E, m, \vartheta),$$

$$\mathcal{K}_2(E, m, \vartheta) := \mathbb{K}(E, m, \mathcal{T}(E, m, \vartheta))\mathcal{T}'_m(E, m, \vartheta),$$

$$\mathcal{S}(E, m, \vartheta) := \mathbb{S}(E, m, \mathcal{T}(E, m, \vartheta)),$$

$$\mathcal{A}_1(E, m, \vartheta) := \mathcal{T}(E, m, \vartheta)\varphi''_{E\theta}(E, m, \mathcal{T}(E, m, \vartheta)) + c_1(E, m, \mathcal{T}(E, m, \vartheta))$$

$$\mathcal{A}_2(E, m, \vartheta) := \mathcal{T}(E, m, \vartheta)\varphi''_{m\theta}(E, m, \mathcal{T}(E, m, \vartheta)) + c_2(E, m, \mathcal{T}(E, m, \vartheta)),$$

$$\sigma_E(E, m, \vartheta) := \varphi'_E(E, m, \mathcal{T}(E, m, \vartheta)),$$

$$\sigma_m(E, m, \vartheta) := \varphi'_m(E, m, \mathcal{T}(E, m, \vartheta)).$$

Then the heat flux transforms to:

$$\begin{aligned} \mathbb{K}(E, m, \theta)\nabla\theta &= \mathbb{K}(E, m, \mathcal{T}(e, \vartheta))\nabla\mathcal{T}(E, m, \vartheta) \\ &= \mathcal{K}_0(E, m, \vartheta)\nabla\vartheta + \mathcal{K}_1(E, m, \vartheta)\nabla E + \mathcal{K}_2(E, m, \vartheta)\nabla m. \end{aligned}$$

Thus, in terms of the 5-tuple (u, m, ϑ, e, h) , the original system transforms to the following 5 equations:

$$\rho \ddot{u} - \operatorname{div} \left(\sigma_E(E(u), m, \vartheta) + \mathbb{D}E(\dot{u}) - \operatorname{div}(C_H \nabla E(u) + \mathbb{D}_H \nabla E(\dot{u})) \right) = f_0 - \mu_0 \nabla h^\top m,$$

$$\alpha \dot{m} - \frac{m \times \dot{m}}{\gamma(|m|)} - \lambda \Delta m + \sigma_m(E(u), m, \vartheta) = p_0 + \mu_0 h,$$

$$\begin{aligned} \dot{\vartheta} - \operatorname{div} \left(\mathcal{K}_0(E(u), m, \vartheta) \nabla \vartheta + \mathcal{K}_1(E(u), m, \vartheta) \nabla E(u) + \mathcal{K}_2(E(u), m, \vartheta) \nabla m \right) \\ = \mathcal{S}(E(u), m, \vartheta) e \cdot e + \mathbb{D}E(\dot{u}) : E(\dot{u}) + \mathbb{D}_H \nabla E(\dot{u}) : \nabla E(\dot{u}) + \alpha |\dot{m}|^2 \\ + \mathcal{A}_1(E(u), m, \vartheta) : E(\dot{u}) + \mathcal{A}_2(E(u), m, \vartheta) \cdot \dot{m}, \end{aligned}$$

$$\mu_0 (\dot{h} + \dot{m}) + \operatorname{curl} e = -\mu_0 \nabla m \dot{u} - \mu_0 (\operatorname{div} \dot{u}) m,$$

$$\operatorname{curl} h - \mathcal{S}(E(u), m, \vartheta) e = 0,$$

Pinning effects: phase field $\chi = \chi(E(u), m)$ and **additional dissipation** $\zeta(\dot{\chi})$. Thus, in terms of the 6-tuple $(u, m, \vartheta, e, h, \omega)$, the original system expands to the following six equations/inclusion:

$$\rho \ddot{u} - \operatorname{div} \left(\sigma_E(E(u), m, \vartheta) + \mathbb{D}E(\dot{u}) + \chi'_E(E(u), m)^\top \omega - \operatorname{div}(\mathbb{C}_H \nabla E(u) + \mathbb{D}_H \nabla E(\dot{u})) \right) = f_0 - \mu_0 \nabla h^\top m,$$

$$\alpha \dot{m} - \frac{m \times \dot{m}}{\gamma(|m|)} - \lambda \Delta m + \sigma_m(E(u), m, \vartheta) = p_0 + \mu_0 h - \chi'_m(E(u), m)^\top \omega,$$

$$\begin{aligned} \dot{\vartheta} - \operatorname{div} \left(\mathcal{K}_0(E(u), m, \vartheta) \nabla \vartheta + \mathcal{K}_1(E(u), m, \vartheta) \nabla E(u) + \mathcal{K}_2(E(u), m, \vartheta) \nabla m \right) \\ = \mathcal{S}(E(u), m, \vartheta) e \cdot e + \mathbb{D}E(\dot{u}) : E(\dot{u}) + \mathbb{D}_H \nabla E(\dot{u}) : \nabla E(\dot{u}) + \alpha |\dot{m}|^2 \\ + \mathcal{A}_1(E(u), m, \vartheta) : E(\dot{u}) + \mathcal{A}_2(E(u), m, \vartheta) \cdot \dot{m} \\ + \zeta(\chi'_E(E(u), m) E(\dot{u}) + \chi'_m(E(u), m) \dot{m}), \end{aligned}$$

$$\mu_0 (\dot{h} + \dot{m}) + \operatorname{curl} e = -\mu_0 \nabla m \dot{u} - \mu_0 (\operatorname{div} \dot{u}) m,$$

$$\operatorname{curl} h - \mathcal{S}(E(u), m, \vartheta) e = 0,$$

$$\omega \in \partial \zeta(\chi'_E(E(u), m) E(\dot{u}) + \chi'_m(E(u), m) \dot{m}).$$

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