Modelli Matematici
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per Materiali Speciali

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Transizione di fase solido–solido in un sistema meccanico

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Motivation:

Tin/lead solders
solid–solid phase change model
Dreyer–Müller, preprint ’98

Different crystalline structures $\Longrightarrow$
coefficients depending on an order parameter

Ω	domain in $\mathbb{R}^N$ (bdd, smooth, etc.)
$\Gamma_u,\ \Gamma_\sigma$	complementary parts of $\partial\Omega$
$\mathbf{u} = (u_i)$	displacement
χ	order parameter

Elasticity system for $\mathbf{u}$
with coefficients depending on χ
and mixed boundary conditions

coupled with

Cahn–Hilliard type equation for χ
with forcing term depending on $\mathbf{u}$
and Neumann boundary conditions

Initial conditions

Generalities 2

Equilibrium equation for the stress (σ_{ij})

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

Constitutive laws

$$\begin{aligned}
\sigma_{ij} &= C_{ijk\ell}\big(\varepsilon_{k\ell} - \varepsilon^*_{k\ell}\big) \\
C_{ijk\ell} &= C_{ijk\ell}(\mathcal{X}) \quad \text{(usual symm \& ellip)} \\
\varepsilon_{k\ell} &= \frac{1}{2}\left(\frac{\partial u_k}{\partial x_\ell} + \frac{\partial u_\ell}{\partial x_k}\right) \\
\varepsilon^*_{k\ell} &= \varepsilon^*_{k\ell}(\mathcal{X})
\end{aligned}$$

($\varepsilon^*_{k\ell}$) is the "eigenstrain" due to phase transition

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Boundary conditions

$$\begin{aligned}
u_i &= \text{given} && \text{on } \Gamma_u \\
\sigma_{ij} n_j &= \text{given} && \text{on } \Gamma_\sigma
\end{aligned}$$

Cahn–Hilliard type equations

$$\frac{\partial \chi}{\partial t} + \operatorname{div} \mathbf{J} = 0 \tag{1}$$

$$\mathbf{J} \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \tag{2}$$

$$\mathbf{J} = -M(\chi)\nabla w \qquad (M \text{ elliptic})$$

From (1–2) we deduce

$$\frac{d}{dt}\int_\Omega \chi\, dx = \int_\Omega \frac{\partial \chi}{\partial t}\, dx = 0$$

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constitutive equation for w
(whence supplementary BC)
initial condition for χ

Equations for χ 4

$$
\begin{aligned}
w &= w_1 + w_2 + w_3 \\
w_1 &= -a_{k\ell}\frac{\partial^2 \chi}{\partial x_k \partial x_\ell} \\
&\quad a_{k\ell} = a_{k\ell}(\chi) \quad \text{(elliptic)} \\
w_2 &= \frac{\partial \Psi}{\partial \chi} \qquad (\Psi \text{ is a double well potential}) \\
w_3 &= \frac{\partial}{\partial \chi}\left(\frac{1}{2}\big(\varepsilon_{ij} - \varepsilon^*_{ij}\big) C_{ijk\ell}\big(\varepsilon_{k\ell} - \varepsilon^*_{k\ell}\big)\right) \\
\frac{\partial \chi}{\partial n} &= 0 \qquad \text{on } \partial\Omega
\end{aligned}
$$

Hence

$$
\begin{aligned}
w_3 &= w_{31} + w_{32} \qquad \text{where} \\
w_{31} &= -\sigma_{k\ell}\frac{\partial \varepsilon^*_{k\ell}}{\partial \chi} \\
w_{32} &= \frac{1}{2}\big(\varepsilon_{ij} - \varepsilon^*_{ij}\big)\frac{\partial C_{ijk\ell}}{\partial \chi}\big(\varepsilon_{k\ell} - \varepsilon^*_{k\ell}\big)
\end{aligned}
$$

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0$$
$$\sigma_{ij} = C_{ijk\ell}(\chi)\big(\varepsilon_{k\ell} - \varepsilon^*_{k\ell}(\chi)\big)$$
$$\varepsilon_{k\ell} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_\ell} + \frac{\partial u_\ell}{\partial x_k}\right)$$
$$\frac{\partial \chi}{\partial t} + \operatorname{div}\mathbf{J} = 0$$
$$\mathbf{J} = -M(\chi)\nabla w$$
$$w = w_1 + w_2 + w_{31} + w_{32}$$
$$w_1 = -a_{k\ell}(\chi)\frac{\partial^2 \chi}{\partial x_k \partial x_\ell}$$
$$w_2 = \frac{\partial \Psi}{\partial \chi}$$
$$w_{31} = -\sigma_{k\ell}\frac{\partial \varepsilon^*_{k\ell}}{\partial \chi}$$
$$w_{32} = \frac{1}{2}\big(\varepsilon_{ij} - \varepsilon^*_{ij}\big)\frac{\partial C_{ijk\ell}}{\partial \chi}\big(\varepsilon_{k\ell} - \varepsilon^*_{k\ell}\big)$$

boundary conditions as above
initial condition for χ

Too difficult: no results.

A significant paper: Garcke's abilitation thesis

very general multiphase model: it contains the above problem but some quantities do not depend on χ.

We modify in a different way, as shown below.

Simplification/relaxation:

$M(\chi) \quad \longrightarrow \quad$ identity matrix

$(a_{k\ell}(\chi)) \quad \longrightarrow \quad$ scalar $a(\chi)$

$\eta_{ijk\ell} := \dfrac{\partial C_{ijk\ell}(\chi)}{\partial \chi}$ constant

$w = \mu \dfrac{\partial \chi}{\partial t} +$ previous $w, \qquad \mu > 0$

Constraint:

$\underline{\chi} \le \chi \le \overline{\chi}$ say $0 \le \chi \le 1$

$$
\begin{aligned}
&\operatorname{div}\big(k(\chi)\nabla u - \mathbf{y}(\chi)\big) = 0\\
&\frac{\partial \chi}{\partial t} - \Delta w = 0\\
&w \in \frac{\partial \chi}{\partial t} - a(\chi)\Delta\chi\\
&\quad + \beta(\chi) + \gamma(\chi) + \mathbf{z}(\chi)\cdot\nabla u + \eta|\nabla u|^2
\end{aligned}
$$

initial and boundary conditions

- β maximal monotone in $\mathbb{R}^2$ and $D(\beta) = [0,1]$
- $k, \mathbf{y}, a, \gamma, \mathbf{z}$ Lipschitz functions of χ
- $\inf_{[0,1]} k = k_0 > 0$ and $\inf_{[0,1]} a = a_0 > 0$
- $\eta = \partial k/\partial\chi \in \mathbb{R}$

A little more precise and better organized

$$\left.\begin{aligned} &\operatorname{div}\bigl(k(\chi)\nabla u - \mathbf{y}(\chi)\bigr) = 0 && \\ &u = 0 && \text{on } \Gamma_u \\ &\bigl(k(\chi)\nabla u - \mathbf{y}(\chi)\bigr)\cdot\mathbf{n} = 0 && \text{on } \Gamma_\sigma \end{aligned}\right\} \quad (1)$$

$$\left.\begin{aligned} &\frac{\partial\chi}{\partial t} - \Delta w = 0 && \\ &w = \frac{\partial\chi}{\partial t} - a(\chi)\Delta\chi + \xi && \\ &\quad + \gamma(\chi) + \mathbf{z}(\chi)\cdot\nabla u + \eta|\nabla u|^2 && \\ &\xi \in \beta(\chi) && \\ &\partial_n w = 0 && \text{on } \partial\Omega \\ &\partial_n \chi = 0 && \text{on } \partial\Omega \\ &\chi(0) = \chi_0 && \end{aligned}\right\} \quad (2)$$

Existence theorem.

Assumptions as above. Moreover

either (i) $N = 1$ *or (ii)* $N = 2$ *and* $\eta = 0$

$$\sup |a'| < a_0 := \inf a$$

$$\chi_0 \in H^1(\Omega), \quad 0 \le \chi_0 \le 1, \quad 0 < \chi^* < 1$$

where χ^* *is the mean value of* χ_0.

Then existence of a solution (u, χ, ξ, w) *with*

$$u \in L^\infty(0, T; H^1(\Omega))$$
$$\chi \in H^1(0, T; L^2(\Omega)) \cap L^2(0, T; H^2(\Omega))$$
$$\xi \in L^2(Q), \quad Q = \Omega \times (0, T)$$
$$w \in L^2(0, T; H^2(\Omega))$$

Uniqueness means

$(u_i, \chi_i, \xi_i, w_i)$ solutions for $i = 1, 2$
then $\quad (u_1, \chi_1) = (u_2, \chi_2)$

Uniqueness theorem.

(i) uniqueness if $N = 1$

(ii) uniqueness if $N = 2$ *among the solutions such that*

$$\iint_Q |\nabla u|^4 dx\, dt < \infty \tag{1}$$

(iii) uniqueness among all the solutions if $N = 2$, $\eta = 0$, *and* (1) *holds for at least a solution.*

Fixed point of the map $\mathcal{F} = \mathcal{F}_2 \circ \mathcal{F}_1$:

$$\chi \quad \overset{\mathcal{F}_1}{\longmapsto} \quad u \quad \overset{\mathcal{F}_2}{\longmapsto} \quad \chi$$

$$\mathcal{F}_1 = \text{ find } u \text{ from (1) with a given } \chi$$

$$\mathcal{F}_2 = \text{ find } \chi \text{ from (2) with a given } u$$

Schauder's theorem:

- Choice of the functional framework
- Continuity of $\mathcal{F}$
- Relative compactness of its range

$$V = \{v \in H^1(\Omega) : \; v = 0 \text{ on } \Gamma_u\}$$

$$\mathcal{V} = L^2(0,T;V) \quad \text{(space for } u\text{)}$$

$$\mathcal{X} = L^2(0,T;H^1(\Omega)) \quad \text{(space for } \chi\text{)}$$

$$\mathcal{K} = \mathcal{K}_R = \{\chi \in \mathcal{X} : \; \chi \in [0,1], \; \|\chi\|_{\mathcal{X}} \le R\}$$

$(R > 0$ properly chosen)

Variational formulation of (1)**:**

$$V = \{v \in H^1(\Omega) : \ v = 0 \text{ on } \Gamma_u\}$$
$$\|v\|^2 = \int_\Omega |\nabla v|^2$$

Fix t and find $u \in V$ such that

$$\int_\Omega \big(k(\chi)\nabla u - \mathbf{y}(\chi)\big) \cdot \nabla v = 0 \qquad \forall\, v \in V$$

Existence and uniqueness

Basic estimate $(v = u)$**:**

$$k_0 \, \|u\|^2 \leq \|u\| \ |\Omega|^{1/2} \sup_{[0,1]} |\mathbf{y}|$$

where $k_0 := \inf_{[0,1]} k$, i.e.

$$\|u\| \leq \frac{1}{k_0} |\Omega|^{1/2} \sup_{[0,1]} |\mathbf{y}|$$

Conclusion for $u = \mathcal{F}_1(\chi)$ with $\chi \in \mathcal{K}_R$:

$$\|u\|_{L^\infty(0,T;H^1(\Omega))} \leq \widehat{C} \tag{1}$$

where $\widehat{C}$ is independent of χ and R.

Continuity of $\mathcal{F}_1 : \mathcal{K}_R \to \mathcal{V}$:

Assumptions:
$\chi_n, \chi \in \mathcal{K}_R$ and $\chi_n \to \chi$ strongly in $\mathcal{X}$

Aim:
$u_n := \mathcal{F}_1(\chi_n) \to u := \mathcal{F}_1(\chi)$ strongly in $\mathcal{V}$

Choose $v = u_n(t) - u(t)$ and integrate over $(0, T)$:

$$
\begin{aligned}
&k_0 \|u_n - u\|_{\mathcal{V}}^2 \leq \iint_Q k(\chi_n) |\nabla(u_n - u)|^2 \\
&= \iint_Q \big(\mathbf{y}(\chi_n) - \mathbf{y}(\chi)\big) \cdot \nabla(u_n - u) \\
&\quad + \iint_Q \big(k(\chi) - k(\chi_n)\big) \nabla u \cdot \nabla(u_n - u) \\
&\leq c \|\mathbf{y}(\chi_n) - \mathbf{y}(\chi)\|_{L^2(Q)} \\
&\quad + c \|\nabla u\|_{L^p(Q)} \|k(\chi) - k(\chi_n)\|_{L^q(Q)} \\
&\text{where} \quad c = 2T^{1/2} \widehat{C} \quad \text{and} \quad \frac{1}{p} + \frac{1}{q} + \frac{1}{2} = 1.
\end{aligned}
$$

Hence, a Meyers type result is needed:
Zafran, J. Funct. Anal. 1980 (general result)

$$\mathcal{F}_2 : \big(\mathcal{F}_1(\mathcal{K}_R) \subseteq\big)\, \widehat{\mathcal{U}} \to \mathcal{K}_R, \quad u \mapsto \chi$$

$$\widehat{\mathcal{U}} = \Big\{ v \in \mathcal{V} : \|v\|_{L^\infty(0,T;H^1(\Omega))} \le \widehat{C} \Big\}$$

$\widehat{C}$ given by the basic estimate

$V = \{ v \in H^1(\Omega) : \; v = 0 \text{ su } \Gamma_0 \}$

$\mathcal{V} = L^2(0,T;V)$

$\mathcal{X} := L^2(0,T;H^1(\Omega))$

$\mathcal{K}_R = \{ \chi \in \mathcal{X} : \; \chi \in [0,1], \; \|\chi\|_{\mathcal{X}} \le R \}$

- existence of χ
- uniqueness of χ
- $\chi \in \mathcal{K}_R$ for R large enough
- $\mathcal{F}_2$ is continuous
- $\mathcal{F}_2(\widehat{\mathcal{U}})$ is relatively compact in $\mathcal{X}$

$$
\begin{aligned}
&\frac{\partial \chi}{\partial t} - \Delta w = 0 \\
&w \in \frac{\partial \chi}{\partial t} - a(\chi)\Delta\chi + \beta(\chi) + \gamma(\chi) \\
&\quad + \mathbf{z}(\chi) \cdot \nabla u + \eta |\nabla u|^2 \\
&\partial_n \chi = \partial_n w = 0 \qquad \text{on } \partial\Omega \\
&\chi(0) = \chi_0
\end{aligned}
$$

Abstract formulation:

$$
\begin{aligned}
&H^1(\Omega) \subset L^2(\Omega) \subset H^1(\Omega)' \\
&A : H^1(\Omega) \to H^1(\Omega)' \\
&\langle A\varphi, v\rangle = \int_\Omega \nabla\varphi \cdot \nabla v \quad \forall\, \varphi, v \in H^1(\Omega) \\
&\chi' + Aw = 0 \\
&w \in \chi' + a(\chi)\, A\chi + \beta(\chi) + \gamma(\chi) \\
&\quad + \mathbf{z}(\chi) \cdot \nabla u + \eta |\nabla u|^2 \\
&\chi(0) = \chi_0
\end{aligned}
$$

Trouble:
we need $\eta|\nabla u|^2 \in L^2(Q)$
Hence, **either** 1D **or** $\eta = 0$.

- Yosida regularization β_ε
- as constraints are lost, take proper extensions of $a, \gamma, \mathbf{z}$ with $a \geq a_0 > 0$
- limit as $\varepsilon \to 0$

After a Galerkin approximation
we have a solution $(\chi, w) = (\chi_\varepsilon, w_\varepsilon)$ to

$$\begin{aligned}
&\chi' + Aw = 0 \\
&w = \chi' + a(\chi)\, A\chi + \beta_\varepsilon(\chi) + \gamma(\chi) \\
&\quad + \mathbf{z}(\chi) \cdot \nabla u + \eta |\nabla u|^2 \\
&\chi(0) = \chi_0
\end{aligned}$$

Main tool for a priori estimates:

$$X_0 := \left\{ v \in H^1(\Omega) : \int_\Omega v = 0 \right\}$$
$$X_0' := \left\{ f \in H^1(\Omega)' : \langle f, 1 \rangle = 0 \right\}$$

Then

$A|_{X_0} : X_0 \xrightarrow{\text{iso}} X_0'$. Set $\mathcal{N} := \{A|_{X_0}\}^{-1}$
i.e., $\mathcal{N}$ solves generalized Neumann problems

$$\chi^* := \frac{1}{|\Omega|} \int_\Omega \chi_0 = \frac{1}{|\Omega|} \int_\Omega \chi(t) \quad \forall t$$
$$\int_\Omega \frac{\partial \chi}{\partial t} = 0 \quad \forall t$$

at least formally.

More precisely

$\chi(t) - \chi^*$ and $\chi'(t)$ belong to X_0' $\forall t$

First a priori estimate:

$$\chi' + Aw = 0 \qquad \times\, \mathcal{N}(\chi - \chi^*)$$

$$\left.\begin{aligned} w = \chi' + \overbrace{a(\chi)\, A\chi}^{\text{bad}} + \beta_\varepsilon(\chi) + \gamma(\chi) \\ + \mathbf{z}(\chi)\cdot\nabla u + \eta|\nabla u|^2 \end{aligned}\right\} \times (\chi - \chi^*)$$

and integrate the difference over $(0,t)$.

$$\langle a(\chi)A(\chi), \chi - \chi^*\rangle = \int_\Omega \nabla\chi \cdot \nabla\big(a(\chi)(\chi - \chi^*)\big)$$

$$\geq a_0 \iint_{Q_t} |\nabla\chi|^2 - \sup|a'| \iint_{Q_t} |\nabla\chi|^2$$

That is why we assume $\sup|a'| < a_0$.

We get

$$\|\chi_\varepsilon\|_{\mathcal{X}\cap L^\infty(0,T;L^2(\Omega))} \leq \widetilde{C}$$

Choose here

$$R > \widetilde{C} \quad \text{and} \quad \mathcal{K} = \mathcal{K}_R$$

Dealing with the limit

- The above estimate yields some weak convergence.
- However, due to the nonlinear terms, some stronger convergence is needed. This is given by further a priori estimates

$$\|\chi_\varepsilon\|_{L^\infty(0,T;H^1(\Omega))\cap L^2(0,T;H^2(\Omega))} \leq c$$

$$\|\chi_\varepsilon'\|_{L^2(Q)} \leq c$$

$$\|\beta_\varepsilon(\chi_\varepsilon)\|_{L^2(Q)} \leq c$$

$$\|w_\varepsilon\|_{L^2(0,T;H^2(\Omega))} \leq c$$

All this yields

- limit as $\varepsilon \to 0$
- existence of χ

Provided χ is **unique**, we have also:

- $\mathcal{F}_2$ is well defined and
- estimates for $\mathcal{F}_2(\widehat{\mathcal{U}})$ relatively compact
- estimates for $\mathcal{F}_2$ continuous

$(\chi_i, \xi_i, w_i) =$ two solutions
and $\chi := \chi_1 - \chi_2$, etc.

$$\left.\begin{array}{l}\text{difference of}\\ \chi_i' + Aw_i = 0\end{array}\right\} \qquad \times \mathcal{N}\chi$$

$$\left.\begin{array}{l}\text{difference of}\\ w_i = \chi_i' + a(\chi_i)\, A\chi_i + \xi_i\\ \quad + \gamma(\chi_i) + \mathbf{z}(\chi_i)\cdot\nabla u + \eta|\nabla u|^2\end{array}\right\} \qquad \times \chi$$

and integrate the difference over $(0, t)$.

- in the difference no $\eta -$ term
- worst terms: with a and $\mathbf{z}$
- set $a_i := a(\chi_i)$
- set $a_i' := a'(\chi_i)$

Left hand side:

$$\frac{1}{2}\|\chi(t)\|_{L^2}^2 + (\geq 0) + \int_0^t \underbrace{\int_\Omega \nabla\chi\cdot\nabla(a_1\chi)}_{\text{bad}}$$

$$\begin{aligned}\text{bad} &= \int_\Omega a_1|\nabla\chi|^2 + \int_\Omega a_1'\,\chi\,\nabla\chi_1\cdot\nabla\chi \\ &\geq a_0\|\nabla\chi\|_{L^2}^2 - c\|\nabla\chi_1\|_{L^4}\|\chi\|_{L^4}\|\nabla\chi\|_{L^2} \\ &\geq \frac{a_0}{2}\|\nabla\chi\|_{L^2}^2 - c\|\nabla\chi_1\|_{L^4}^2\|\chi\|_{L^4}^2\end{aligned}$$

$$\begin{aligned}&\|\nabla\chi_1\|_{L^4}^2\|\chi\|_{L^4}^2 \\ \text{GN 2D} \Rightarrow\quad &\leq c\|\chi_1\|_{L^\infty}\|\chi_1\|_{H^2}\cdot\|\chi\|_{L^2}\|\nabla\chi\|_{L^2} \\ &\leq \delta\|\nabla\chi\|_{L^2}^2 + C_\delta\underbrace{\|\chi_1\|_{H^2}^2}_{\in L^1(0,T)}\|\chi\|_{L^2}^2\end{aligned}$$

$$\Downarrow$$

Gronwall

... on the left hand side

$$\|\chi(t)\|_{L^2}^2 + \int_0^t \|\nabla\chi\|_{L^2}^2 + \dots$$

with some small coefficients

On the right hand side:

$$\text{bad} = \int_0^t \underbrace{\big(c_{\mathbf{z}} \|\nabla u\|_{L^2} \|\chi\|_{L^4}^2 + \langle A\chi_2, (a_2 - a_1)\chi\rangle\big)}_{\leq c(\|\nabla u\|_{L^2} + \|A\chi_2\|_{L^2}) \|\chi\|_{L^4}^2}$$

(GN 2D again)

$$\leq c \int_0^t \big(\|\nabla u\|_{L^2} + \|A\chi_2\|_{L^2}\big) \|\chi\|_{L^2} \|\nabla\chi\|_{L^2}$$

$$\leq \delta \int_0^t \|\nabla\chi\|_{L^2}^2$$

$$+ C_\delta \int_0^t \underbrace{\big(\|u\|_{H^1}^2 + \|\chi_2\|_{H^2}^2\big)}_{\in L^1(0,T)} \|\chi\|_{L^2}^2$$

$$\Downarrow$$

Gronwall

Schauder's theorem applies. Hence:

existence of a solution with

$$u \in L^\infty(0,T;H^1(\Omega))$$

and (χ, ξ, w) according to our a priori estimates

$\chi \in L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))$
since $\|\chi_\varepsilon\|_{L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega))} \leq c$
$\chi \in H^1(0,T;L^2(\Omega))$
since $\|\chi_\varepsilon'\|_{L^2(Q)} \leq c$
$\xi \in L^2(Q)$
since $\|\beta_\varepsilon(\chi_\varepsilon)\|_{L^2(Q)} \leq c$
$w \in L^2(0,T;H^2(\Omega))$
since $\|w_\varepsilon\|_{L^2(0,T;H^2(\Omega))} \leq c$

2D with $\eta \neq 0$ and 3D: **open**