A phase transition model with the possibility of voids

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Aim of the talk

- discuss a phase transition model including possibly voids formation
- consider the modelling aspects: to derive the model by
  - choosing the **free energy** (responsible for the thermomechanical equilibrium of the system) and the **pseudo-potential of dissipation** (responsible for the thermomechanical evolution of the system)
  - introducing the **constitutive relations** and the **basic laws of continuum mechanics**
- consider the analytical aspects: to point out the EXISTENCE AND UNIQUENESS OF SOLUTIONS for the related PDE'S SYSTEM
- to introduce some open related problems like the possibility to apply this kind of approach to SHAPE MEMORY ALLOYS

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Phase transitions

Phase-field models means deriving equations for:

- ϑ the absolute temperature (entropy balance equation)
- ε the linearized symmetric strain tensor (quasi-static macroscopic equation of motion)
- $\boldsymbol{\beta} = (\beta_1, \beta_2)^\tau$ where β_1 and β_2 the volume fraction of the two phases (microscopic equation of motion)

Example

The mass balance

- Assume the same constant density ρ and the same velocity $\boldsymbol{U} := \boldsymbol{u}_t$ (being $\mathbf{u} = (u_1, u_2, u_3)$ the small displacement) for liquid and solid phases.

Then, the mass balance can be written as

$$\frac{d}{dt}\left[\rho(\beta_1+\beta_2)\right] + \rho(\beta_1+\beta_2)\,\mathrm{div}\,\boldsymbol{U} = 0 \quad \text{in } Q := \Omega \times (0,T).$$

Moreover, within the small perturbations assumption, it gives

$$\partial_t(\beta_1+\beta_2) + (\beta_1^0+\beta_2^0)\,\mathrm{div}\,\boldsymbol{U} = 0 \quad \text{in } Q. \qquad \text{(MB)}$$

Take the reference value of the material volume fraction $\beta_1^0+\beta_2^0 = 1$ for simplicity.

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The free energy

The free energy functional must include the constraint on $\boldsymbol{\beta}$, i.e. it is

$$\Psi = -\vartheta \ln \vartheta + \frac{1}{2}|\varepsilon(\boldsymbol{u})|^2 - \frac{\ell}{\vartheta_c}(\vartheta - \vartheta_c)\beta_1 + I_K(\boldsymbol{\beta}) + \frac{1}{2}|\nabla \boldsymbol{\beta}|^2$$

where $\varepsilon(\mathbf{u}) := (u_{i,j} + u_{j,i})/2$ $(i, j = 1, 2, 3)$ is the linearized symmetric strain tensor, $\ell > 0$ is the latent heat at the phase change temperature ϑ_c, $\nabla\beta_1$ describes properties of the voids-liquid ($\nabla\beta_2$ of the voids-solid) interface.
I_K is the indicator function of the convex set

$$K := \{(\beta_1, \beta_2) \in \mathbb{R}^2 \text{ such that } \beta_1, \beta_2, \beta_1 + \beta_2 \in [0, 1]\},$$

that is

$$I_K(x) = \begin{cases} 0 & \text{if } x \in K \\ +\infty & \text{otherwise.} \end{cases}$$

Return to B snd H

The pseudo-potential of dissipation

We include dissipation by following the approach of [Moreau, 1971]

$$\Phi(\nabla\vartheta, \dot{\boldsymbol{\beta}}, \nabla\dot{\boldsymbol{\beta}}, \varepsilon(\boldsymbol{u}_t)) = \frac{1}{2\vartheta}|\nabla\vartheta|^2 + \frac{1}{2}|\dot{\boldsymbol{\beta}}|^2 + \frac{1}{2}|\nabla\dot{\boldsymbol{\beta}}|^2 + \frac{1}{2}|\varepsilon(\boldsymbol{u}_t)|^2 + I_0\big(\partial_t(\beta_1+\beta_2) + \operatorname{div}\mathbf{u}_t\big),$$

where the presence of $1/\vartheta$ entails that thermal dissipation becomes more relevant at low temperatures: indeed it is more difficult to heat a hot body than a cold one.
The function I_0 is the indicator function of 0, i.e.

$$I_0(x) = \begin{cases} 0 & \text{if } x = 0 \\ +\infty & \text{otherwise.} \end{cases}$$

Return to σ

Return to B snd H

Remark 1

From basic laws of Thermodynamics and Constitutive relations

we deduce...

- The equation of macroscopic motion $\Rightarrow \varepsilon(\mathbf{u})$
- The equation of microscopic motion $\Rightarrow \boldsymbol{\beta} = (\beta_1, \beta_2)^\tau$ both deduced from the generalized principle of virtual power (cf. [M. Frémond, 2002])
- The entropy balance equation $\Rightarrow \vartheta$

Equation of macroscopic motion

The quasi-static macroscopic equation of motion is provided by the principle of virtual power and it is

$$\begin{aligned} \operatorname{div}\sigma + \boldsymbol{f} &= \mathbf{0} \quad \text{in } Q \\ \sigma \cdot \boldsymbol{n} &= \hat{\boldsymbol{g}} \quad \text{on } \Sigma := \partial\Omega \times (0, T), \end{aligned}$$

σ is the stress variable, $\boldsymbol{f}$ = exterior volume force, $\hat{\boldsymbol{g}}$ = exterior contact force on the boundary.

Due to Consitutive Laws

the equilibrium equation can be rewritten as

$$\boxed{\operatorname{div}\left(\varepsilon(\boldsymbol{u}) + \varepsilon(\boldsymbol{u}_t) - p\mathbb{I}\right) + \boldsymbol{f} = \mathbf{0} \quad \text{in } Q,} \qquad \text{(m)}$$

where

$$-p \in \partial I_0\left(\partial_t(\beta_1 + \beta_2) + \operatorname{div}\boldsymbol{u}_t\right)$$

represents just the PRESSURE of the system!

The equation of microscopic motion

The balance of momentum for microscopic forces, derived from a generalization (cf. [M. Frémond, 2002]) of the principle of virtual power (in absence of external actions), is

$$\boldsymbol{B} - \operatorname{div} H = \mathbf{0} \quad \text{in Q}, \qquad H \cdot \boldsymbol{n} = 0 \quad \text{on } \Sigma.$$

Due to the standard consititutive laws Consitutive Laws, H (an energy flux tensor) and $\boldsymbol{B}$ (a density of energy vector), representing internal microscopic forces, we have

$$\dot{\beta} - \Delta\dot{\beta} - \Delta\beta + \xi - p\mathbf{1} = \begin{pmatrix} \frac{\ell}{\vartheta_c}(\vartheta - \vartheta_c) \\ 0 \end{pmatrix} \text{ in } Q \qquad (M)$$

$$\partial_{\boldsymbol{n}}\dot{\beta} = \partial_{\boldsymbol{n}}\beta = 0 \quad \text{on } \Sigma,$$

where $\xi \in \partial I_K(\beta)$ and $-p \in \partial I_0\big(\partial_t(\beta_1 + \beta_2) + \operatorname{div} \mathbf{u}_t\big)$.

Physical Examples

Energy-Entropy balance

The small perturbations assumption allows to neglect the dissipative contributions on the right hand side and due to the fact that absolute temperature $\vartheta > 0$, the energy balance equation ◂ Energy balance

$$\vartheta \left(s_t + \operatorname{div} \mathbf{Q} - \frac{r}{\vartheta} \right) = (\mathbf{B}^d, H^d, -\mathbf{Q}^d) \cdot (\dot{\beta}, \nabla\dot{\beta}, \nabla\vartheta) (= 0)$$

reduces to the entropy balance ($R = r/\vartheta$)

$$\boxed{s_t + \operatorname{div} \mathbf{Q} = R.}$$

Finally, since $s = -\frac{\partial\Psi}{\partial\vartheta}$ and $\mathbf{Q} = -\frac{\partial\Phi}{\partial\nabla\vartheta}$, with our choice of Ψ and Φ, it becomes:

$$\boxed{\partial_t(\ln\vartheta) + \frac{\ell}{\vartheta_c}\partial_t\beta_1 - \Delta(\ln\vartheta) = R \quad \text{in } Q.} \qquad \text{(E)}$$

Problem (P)

Find suitably regular $(\mathbf{u},\, \vartheta,\, \beta_1, \beta_2)$ s.t.

$$\operatorname{div}\left(\varepsilon(\boldsymbol{u}) + \varepsilon(\boldsymbol{u}_t) - p\mathbb{I}\right) + \boldsymbol{f} = \mathbf{0} \quad \text{in } Q, \qquad (m)$$

$$-p \in \partial I_0(\partial_t(\beta_1 + \beta_2) + \operatorname{div} \mathbf{u}_t) \quad \text{in } Q,$$

$$\partial_t(\ln\vartheta) + \frac{\ell}{\vartheta_c}\partial_t\beta_1 - \Delta(\ln\vartheta) = R \quad \text{in } Q, \qquad (E)$$

$$\dot{\boldsymbol{\beta}} - \Delta(\dot{\boldsymbol{\beta}} + \boldsymbol{\beta}) + \boldsymbol{\xi} - p\mathbf{1} = \begin{pmatrix} \frac{\ell}{\vartheta_c}(\vartheta - \vartheta_c) \\ 0 \end{pmatrix} \quad \text{in } Q, \qquad (M)$$

$$\boldsymbol{\xi} = (\xi_1, \xi_2) \in \partial I_K(\boldsymbol{\beta}) \quad \text{in } Q$$

$+$ suitable I.C. and B.C.

The global existence result

Theorem 1 [M. Frémond and E. R.]. Take suitable assumptions on the data and let T be a positive final time. Then Problem (P) has at least a solution on the whole time interval $[0, T]$.

▸ Remark 1

▸ Remark 2

The uniqueness result

Theorem 2 [M. Frémond and E. R.]. Let T be a positive final time. Besides conditions, which guarantee existence, suppose that

$$\partial I_K(\beta) \text{ is substituted by a function } \alpha \in C^{0,1}(\mathbb{R}^2).$$

Then, the solution of Theorem 1 turns out to be unique and to depend continuously on the data of the problem.

▸ Remark

Some perspectives for the future...

- To treat the case of a fully nonlinear entropy (or energy) balance equation, i.e. without using the assumption of SMALL PERTURBATIONS.
- To get uniqueness of solutions in the general case of the double nonsmooth nonlinearities in the equation of Microscopic motion.
- To consider the problem of the freezing of soil not saturated (there is the possibility of having voids before the phase change occurs and after too).
- To treat the case of phase transitions in the SHAPE MEMORY ALLOYS with the possibility of voids.

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Idea of the uniqueness' proof

- Make the following tests:
  - $(E^1 - E^2)$ with $2(\ln\vartheta^1 - \ln\vartheta^2)$;
  - $(m^1 - m^2)$ with $2(\mathbf{u}^1 - \mathbf{u}^2)_t$;
  - $(M^1 - M^2)$ with $((\beta_1^1)_t - (\beta_1^2)_t, (\beta_2^1)_t - (\beta_2^2)_t)$;
- use α is Lipschitz continuous for the term $\int_0^t |\alpha(\chi^1) - \alpha(\chi^2)|_{L^2(\Omega)} |(\chi^1)_t - (\chi^2)_t|_{L^2(\Omega)}$;
- note that $\gamma : w \to \exp w$, is a locally Lipschitz continuous function, $\vartheta^i = \gamma(\ln\vartheta^i)$, and $\ln\vartheta^i$ are bounded in $L^\infty(Q)$ for $i = 1, 2$, hence

$$|\vartheta^1 - \vartheta^2|_{L^2(\Omega)} \le c_{\gamma, |\ln\vartheta^i|_{L^\infty(Q)}} |\ln\vartheta^1 - \ln\vartheta^2|_{L^2(\Omega)}.$$

Hence, thanks to the regularity $L^\infty(Q)$ of $\ln\vartheta^i$, we are able to get the desired continuous dependence estimate, entailing, in particular, uniqueness of solutions to Problem (P).

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Phase transitions

...an example: the melting-solidification process in a bounded domain $\Omega \subset \mathbb{R}^3$ with regular boundary, e.g., containing cast iron or ice. It contains bubbles or VOIDS. They result from the solidification of a liquid phase without voids $\Longrightarrow$
voids have been created during the phase change

The column vector of volume fractions $\boldsymbol{\beta} = (\beta_1, \beta_2)^\tau$:

- $\beta_1 \in [0, 1]$: the liquid volume fraction
- $\beta_2 \in [0, 1]$: the solid volume fraction
- $1 - \beta_1 - \beta_2$: the void volume fraction.

We do not have the relation $\beta_1 + \beta_2 = 1$ but only $\beta_1 + \beta_2 \leq 1$ because we may have voids but no interpenetration

Return

The pseudo-potential of dissipation

The term $I_0\left(\partial_t(\beta_1 + \beta_2) + \operatorname{div} \mathbf{u}_t\right)$ in Φ is zero if (MB) is satisfied and it is $+\infty$ otherwise, where

$$\partial_t(\beta_1 + \beta_2) + \operatorname{div} \boldsymbol{u}_t = 0 \quad \text{in } Q. \tag{MB}$$

Return

From basic laws of Thermodynamics and Constitutive relations

Principle of virtual power for microscopic motion

For any subdomain $D \subset \Omega$ and any virtual microscopic velocity v,

$$P_{\text{int}}(D, \mathbf{v}) + P_{\text{ext}}(D, \mathbf{v}) = \mathbf{0},$$

where ($\mathbf{B}$ and H new interior forces)

$$P_{\text{int}}(D, \mathbf{v}) := -\int_D (\mathbf{B} \cdot \mathbf{v} + H : \nabla \mathbf{v}),$$

$$P_{\text{ext}}(D, \mathbf{v}) := \int_D \mathbf{A} \cdot \mathbf{v} + \int_{\partial D} \mathbf{a} \cdot \mathbf{v} = 0.$$

From which (in absence of external actions) we derive an equilibrium equation in Ω

$$\boxed{\mathbf{B} - \operatorname{div} H = \mathbf{0}}$$

with the natural associated boundary condition on $\partial\Omega$

$$H \cdot \boldsymbol{n} = 0.$$

Return

Constitutive laws...

The stress tensor $\sigma = \sigma^{nd} + \sigma^{d}$

- $\sigma^{nd} = \frac{\partial \Psi}{\partial \varepsilon(\boldsymbol{u})} = \varepsilon(\boldsymbol{u})$
- $\sigma^{d} = \frac{\partial \Phi}{\partial \varepsilon(\boldsymbol{u}_t)} = \varepsilon(\boldsymbol{u}_t) - p\mathbb{I}$.

where $-p$ is a selection of ∂I_0 and because the of the choice of the Free energy and of the Pseudo-potential of dissipation

Pseudopotential

Return

Constitutive laws

The interior forces

- $\mathbf{B} = \mathbf{B}^{nd} + \mathbf{B}^{d}$ (a density of energy vector)
  - $\mathbf{B}^{nd} = \frac{\partial \Psi}{\partial \boldsymbol{\beta}} = -\begin{pmatrix} \frac{\ell}{\vartheta_c}(\vartheta - \vartheta_c) \\ 0 \end{pmatrix} + \xi,$
  - $\mathbf{B}^{d} = \frac{\partial \Phi}{\partial \dot{\boldsymbol{\beta}}} = \dot{\boldsymbol{\beta}} - p\mathbf{1};$
- $H = H^{nd} + H^{d}$ (an energy flux tensor)
  - $H^{nd} = \frac{\partial \Psi}{\partial \nabla \boldsymbol{\beta}} = \nabla \boldsymbol{\beta},$
  - $H^{d} = \frac{\partial \Phi}{\partial \nabla \dot{\boldsymbol{\beta}}} = \nabla \dot{\boldsymbol{\beta}}.$

where ξ and $-p$ are two selections of ∂I_K and ∂I_0, respectively and
because of the choices of the Free energy

Free energy

and of the Pseudo-potential of dissipation

Pseudopotential

Return

Some physical case covered by the model

Take the case $\beta_1, \beta_2 \in (0,1)$ and $-\Delta\boldsymbol{\beta} = \mathbf{0}$, then we can write (M) M as

$$\dot{\beta}_1 - \Delta\dot{\beta}_1 = p + \vartheta - \vartheta_c \quad \text{in } Q,$$
$$\dot{\chi}_1 - \Delta\dot{\chi}_1 = 2p + \vartheta - \vartheta_c \quad \text{in } Q,$$

where $\chi_1 = \beta_1 + \beta_2$. Hence, we find

- ♢ If $(p + \vartheta - \vartheta_c) < 0$ a.e. in Q, then $\dot{\beta}_1 < 0$ a.e. in Q (think of solid-liquid phase transitions: the liquid content decreases).
- ♢ If $(2p + \vartheta - \vartheta_c) < 0$ a.e. in Q, then $\dot{\chi}_1 = \partial_t(\beta_1 + \beta_2) < 0$ a.e. in Q and, by the mass balance equation, we verify the frost heave phenomenon in soils:

$$\boxed{\operatorname{div} \mathbf{u}_t = -\partial_t(\beta_1 + \beta_2) > 0 \quad \text{a.e. in } Q.}$$

Return

Energy-Entropy balance

As usual the Energy Balance reads

$$e_t + \operatorname{div}\mathbf{q} = r + (\mathbf{B}^d, H^d, -\mathbf{Q}^d)\cdot(\dot{\boldsymbol{\beta}}, \nabla\dot{\boldsymbol{\beta}}, \nabla\vartheta),$$

where e is the *internal energy* , $\mathbf{q}$ the heat flux, r the external rate of heat production.

Using the definition of *entropy* and the Helmoltz relation:

$$s = -\frac{\partial\Psi}{\partial\vartheta}, \quad e = \Psi + \vartheta s,$$

we get

$$\vartheta\left(s_t + \operatorname{div}\mathbf{Q} - \frac{r}{\vartheta}\right) = (\mathbf{B}^d, H^d, -\mathbf{Q}^d)\cdot(\dot{\boldsymbol{\beta}}, \nabla\dot{\boldsymbol{\beta}}, \nabla\vartheta)$$

where $\mathbf{Q} := \mathbf{q}/\vartheta$.

Return

The global existence result

Uniqueness seems to be difficult due to

- the difficult coupling between the microscopic motion (prresence of ϑ) and the entropy balance equations (the variable is $\ln\vartheta$) (cf. also [Bonetti, Colli, Frémond]) and
- the double nonsmooth nonlinearities in the microscopic motion equation: $\partial I_K(\boldsymbol{\beta})$ and $\partial I_0(\partial_t(\beta_1+\beta_2)+\operatorname{div}\mathbf{u}_t)$.

Return

The global existence result

Note that we are able to prove the same existence result for more general maximal monotone graphs, that is if ∂I_K in (M) is substituted by $\alpha := \partial j$ with

$j : \mathbb{R}^2 \to [0, +\infty]$ a proper, convex, lower semicontinuous function such that $j(0) = 0$.

Example. The logarithmic or the polynomial cases.

Return

The uniqueness result

We overcome difficulties due to the difficult coupling between

- the entropy balance equation (E) $\Longrightarrow$ parabolic in $\ln\vartheta$ and
- the microscopic equation of motion (M) $\Longrightarrow$ containing the ϑ variable

using a regularity result for parabolic equations entailing in particular $\ln\vartheta \in L^\infty(Q)$ (cf. [Ladyženskaja, Solonnikov, Uralçeva, 1967]).

Return