

A mathematical model for rate-independent phase transformations with hysteresis*

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1 Introduction

The modeling of phase transformations (PT) in single and poly crystals is important to make the shape memory effect applicable in practical engineering where complex geometries and loading behavior must be considered. There are many mathematical models for hysteretic behavior during uniaxial loading cycles, see e.g. [BrS96, KL*97, KuM98]. Here we want to derive a general model for elastic deformations and PT in three-dimensional bodies.

The different phases in shape memory alloys arise from different possible stress-free arrangements of the crystallographic lattice with nearly the same energies. The number n of phases varies from 2 to 25 depending on the material under consideration. For a fixed time the elastic body decomposes into the n regions associated to each phase. However, these regions typically develop fine microstructure, e.g. laminated twins where each layer has the thickness of only a few atomic distances (cf. [BaJ87, BaJ92]). It is one of the tasks of the mathematical modeling in material science to describe the effective behavior of such phase mixtures on the mesoscopic level.

Our interest lies in deformation processes where the movements of the domain walls (boundaries between the phase regions) is slow and associated to changing external loadings. Thus, we consider a rate-independent model where all inertia terms and the kinetic energy are neglected. Our time $t \in [0, T]$ is a process time and the system behavior is not changed under monotone reparametrizations of the time interval.

The state of a system is described by the elastic deformation and the distribution of the phases. At each point the material can choose to be in one of the n different phases, and changing from phase i into phase j leads to a dissipation of energy which is $\kappa_{i \rightarrow j}$ times the volume of the changed region. Microscopically this energy arises from rearrangements of the atoms at the slowly moving domains walls. Mesoscopically this leads to an energetic threshold for PT. Three-dimensional models for this behavior were

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developed in [Lev95, Lev97] where even the elastoplastic case was considered. Neglecting plastic effects leads to the model which we consider here.

Assume that the body under consideration is given by $\Omega \subset \mathbb{R}^d$. The state of a system is described by the elastic displacement $\mathbf{u} : \Omega \rightarrow \mathbb{R}^d$ and the phase function $c \in \mathcal{P}$, where \mathcal{P} is the set of possible phase functions $c : \Omega \rightarrow \{e_1, \dots, e_n\}$. For rate-independent problems the system is always in elastic equilibrium with respect to the given phases $c(t) \in \mathcal{P}$ and the given external loadings $\mathbf{G}(t)$, viz., $\mathbf{u} = \mathbf{U}(t, c(t))$. Thus, the state of a system is uniquely determined by $c(t)$ and it remains to find an evolution law for the phase distribution.

The extremum principle in [Lev97, Lev98] reduces in our situation to the following two conditions:

- (i) *The process $c : [0, T] \rightarrow \mathcal{P}$ satisfies the total energy balance.*
- (ii) *The state $c(t)$ is stable for all $t \in [0, T]$.*

Stability here means that under given loadings any change of the phase distribution from $c(t)$ to any other $a \in \mathcal{P}$ generates at least as much dissipation as the associated gain in the (elastic) Gibb's energy.

For general loadings \mathbf{G} the existence of a process satisfying (i) and (ii) cannot be guaranteed. In fact, there might be no stable state at all for some given loadings $\mathbf{G}(t)$. This problem arises from the scaling invariance of elasticity which allows the material to form finer and finer microstructure. Thus, any given state c may be unstable with respect to states a having even finer microstructure. See [BaJ87, BaJ92] for the effects for fine microstructure and [BCJ95] for a way to model PT without dissipation.

The goal of the present work is to propose a mathematical way to generate out of the given model a new one which describes the arising microscopical effect on a mesoscopic scale using effective quantities. The general idea is to replace the time-continuous problem by a time-incremental one. For given time increments $0 < t_1 < \dots < t_{n-1} < t_n = T$ we find inductively c_1, c_2, \dots, c_n . Because of the extremum principles at the time level t_k we have to find c_k as minimizer of a functional which depends on the loading $\mathbf{G}(t_k)$ and the previous phase function c_{k-1} . In general this functional does not attain its infimum on \mathcal{P} and it needs to be replaced by a relaxation which is defined on $\widehat{\mathcal{P}}$, which is the closure of the convex hull of \mathcal{P} . Thus, we are lead automatically to a mesoscopic description involving phase mixtures $\widehat{c} \in \widehat{\mathcal{P}}$ rather than pure phases with fine microstructure. This leads to a relaxed incremental problem on $\widehat{\mathcal{P}}$ which always has a solution. Moreover, this incremental problem can be understood as the discretization of a time-continuous relaxed problem which in fact has the same features as the original problem: it is characterized by stability and the energy balance. Similar incremental approaches to rate-independent problems in plasticity are discussed in [CHM99]

One of the important points in this theory is that relaxation gives an automatic algorithm to compute the effective behavior of phase mixtures and we need no further modeling assumptions. In particular, the theory shows that the effective behavior of phase mixtures can be described by a so-called *mixture function* $\widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon})$, see Section 4. This function is analytically defined from stored-energy functions $W_{e_j}(\boldsymbol{\varepsilon})$ of each of the phases. Unfortunately, only in very few cases the formula can be evaluated explicitly (cf. [Bha93, Koh91]), in other cases only certain bounds can be given.

However, we have to note that there is still one point where modelling is important. The relaxation of a single variational problem is well understood but not that of incremental problems, since on each time level we have to deal with minimizing sequences which

depend on the minimizing sequences of the previous time level. For general problems we have to extract the correct informations from the microscopic level which allows us to control the interactions between the microstructures at the different time levels. In this paper we use the simplest possible relaxation which amounts in the fact that we only control the mesoscopically averaged volume fraction of the phases (the weak limit of sequences of phase functions). Thus, we obtain dissipation only if the volume fractions change but not if the underlying microstructure changes with fixed volume fraction. This shortcoming will be compensated for in future investigations. However, in Section 6 we give a case where the simple relaxation is proved to be suitable.

2 The mechanical model

Every material point \mathbf{x} in the body $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, can be in one of n phases, written as $c(\mathbf{x}) = e_j = (0, \dots, 0, 1, 0, \dots, 0)^T$. We denote by $P = \{e_1, \dots, e_n\}$ the set of all phases and by

$$\mathcal{P} = \{ c : \Omega \rightarrow P \mid c \text{ measurable} \}$$

the set of all possible phase functions. The material properties of each phase are given by the energy density $W_{e_j}(\boldsymbol{\varepsilon})$ where $\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$ is the linearized strain tensor. Here we restrict ourselves to linearized elasticity, however there is no conceptual difficulty in generalizing the approach to nonlinear, geometrically exact elasticity, see [MTL98].

The different W_{e_j} are given by

$$W_{e_j}(\boldsymbol{\varepsilon}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \mathbf{d}_j) : \mathbb{E}_j(\boldsymbol{\varepsilon} - \mathbf{d}_j) + \beta_j \quad (2.1)$$

where $\mathbb{E}_j \in \text{Lin}(\mathbb{R}_{\text{sym}}^{d \times d}, \mathbb{R}_{\text{sym}}^{d \times d})$ is the elasticity tensor, $\mathbf{d}_j \in \mathbb{R}_{\text{sym}}^{d \times d}$ the transformation strain and $\beta_j \in \mathbb{R}$ the minimal energy of the j th phase. Often in martensitic phase transformations one assumes $\mathbb{E}_j = \mathbb{E}_n$ where n relates to the austenite phase while $i = 1, \dots, n-1$ relates to the different variants of the martensitic phases which are related to each other by the discrete symmetry group of the crystal (e.g. $n = 13$ for PT from a cubic to a monoclinic lattice). Similarly the energies β_j satisfy $\beta_j = \beta_1$ for $j = 1, \dots, n-1$ where $\beta_1 > \beta_n$ ($\beta_1 < \beta_n$) if we are below (above) the critical temperature. The whole analysis works for general inhomogeneous materials with $W_{e_j}(\mathbf{x}, \boldsymbol{\varepsilon})$ but for notational convenience we restrict ourselves to the homogeneous case.

The process time is denoted by $t \in [0, T]$, and for each t the external loadings are prescribed by $\mathbf{G}(t) = (\mathbf{g}_{\text{vol}}(t, \cdot), \mathbf{g}_{\text{surf}}(t, \cdot))$ such that

$$\langle \mathbf{G}(t), \mathbf{u} \rangle = \int_{\Omega} \mathbf{g}_{\text{vol}}(t, \mathbf{x}) \cdot \mathbf{u}(\mathbf{x}) \, d\mathbf{x} + \int_{\mathbf{x} \in \partial\Omega} \mathbf{g}_{\text{surf}}(t, \mathbf{x}) \cdot \mathbf{u}(\mathbf{x}) \, d\mathbf{a}.$$

Moreover, displacement conditions are prescribed by restricting the set of kinematically admissible deformations. Let $\Gamma \subset \partial\Omega$ be the part of the boundary where Dirichlet conditions are prescribed, then we let $V_{\Gamma} = \{ \mathbf{v} \in H^1(\Omega) \mid \mathbf{v}|_{\Gamma} = 0 \}$. The Dirichlet conditions are given through a smooth function $\boldsymbol{\varphi} : [0, T] \times \bar{\Omega}$ in the form $\mathbf{u}(t, \cdot) \in V(t) \stackrel{\text{def}}{=} \boldsymbol{\varphi}(t, \cdot) + V_{\Gamma}$.

The general assumption for rate-independent processes is that at each time t the system is in elastic equilibrium. This is equivalent to saying that for a given phase function

$c(t)$, loading $\mathbf{G}(t)$ and boundary conditions $\boldsymbol{\varphi}(t)$ the deformation is the unique minimizer of the elastic energy

$$E(t, c, \mathbf{v}) = \int_{\Omega} W_{c(\mathbf{x})}(\boldsymbol{\varepsilon}(\mathbf{v})(\mathbf{x})) \, d\mathbf{x} - \langle \mathbf{G}(t), \mathbf{v} \rangle.$$

Clearly $\mathbf{u} = \arg \min \{ E(t, c, \mathbf{v}) \mid \mathbf{v} \in V(t) \}$ is uniquely determined as $E(t, c, \cdot)$ is quadratic and coercive. We write $\mathbf{u} = \mathbf{U}(t, c)$ to denote this unique solution and call the minimal value

$$I(t, c) = \inf \{ E(t, c, \mathbf{v}) \mid \mathbf{v} \in V(t) \} = E(t, c, \mathbf{U}(t, c))$$

the Gibbs' energy at time t of the phase function $c \in \mathcal{P}$.

A function $c : [0, T] \rightarrow \mathcal{P}$ is called a process and $c(t)$ is called the state of the system at time t . It remains to find suitable rules according to which $c(t)$ evolves. Our basic modeling assumption is that changing the phase function in a region $\omega \subset \Omega$ from phase e_i to phase e_j dissipates the energy $\text{vol}(\omega)\kappa_{i \rightarrow j}$. Here $\kappa_{j \rightarrow j} = 0$, and $\kappa_{i \rightarrow j} > 0$ for $j \neq i$ are the dissipation coefficients for a PT from e_i into e_j . They serve as an energetic threshold which makes PT more difficult. Under the assumptions that at most one PT occurs at each material point the dissipation of a PT from state $a \in \mathcal{P}$ into $c \in \mathcal{P}$ is

$$\mathcal{D}(a, c) = \int_{\Omega} D(a(\mathbf{x}), c(\mathbf{x})) \, d\mathbf{x}, \quad \text{where } D(e_i, e_j) = \kappa_{i \rightarrow j}.$$

The total amount of dissipated energy due to PT in the time interval $[t_1, t_2]$ is denoted by $\text{Diss}(c; t_1, t_2)$ and we have

$$\text{Diss}(c; t_1, t_2) = \sup \left\{ \sum_{j=1}^n \mathcal{D}(c(s_{j-1}), c(s_j)) \mid n \in \mathbb{N}, t_1 \leq s_0 < \dots < s_n < t_2 \right\}.$$

The evolution law for c is derived from two physical principles, namely the stability of the states $c(t)$ for all times t and the energy balance. We say that a state c is *stable at time t* if

$$I(t, a) + \mathcal{D}(c, a) \geq I(t, c) \quad \text{for all } a \in \mathcal{P}.$$

This stability means exactly that there is no PT from the given state $c(t)$ which has a gain in the Gibbs' energy which is larger than the associated dissipation. A process $c : [0, T] \rightarrow \mathcal{P}$ satisfies the *energy balance* if for all t_1, t_2 with $0 \leq t_1 \leq t_2 \leq T$ we have

$$I(t_2, c(t_2)) + \text{Diss}(c; t_1, t_2) = I(t_1, c(t_1)) - \int_{t_1}^{t_2} \langle \dot{\mathbf{G}}(s), \mathbf{u}(s) \rangle \, ds. \quad (2.2)$$

For given initial condition $c_0 \in \mathcal{P}$, loading $\mathbf{G}(t)$ and $V(t)$ the mathematical **time-continuous problem** reads:

(CP) For given $c_0 \in \mathcal{P}$ find a process $c : [0, T] \rightarrow \mathcal{P}$ with $c(0) = c_0$ such that for all t the state $c(t)$ is stable at time t and that the energy balance holds.

3 An incremental formulation

We define an incremental formulation of (CP) which at least formally approaches the time–continuous problem when the time increments tend to 0. The main philosophy is that the incremental problem preserves the two essential features of the mechanics, namely the stability and the energy balance, however, the latter only on a discretized level.

For $0 < t_1 < \dots < t_{N-1} < t_N = T$ we define the **incremental problem**:

(IP) For given c_{k-1} find c_k such that $I(t_k, c_k) + \mathcal{D}(c_{k-1}, c_k)$ is minimal, i.e.

$$c_k = \arg \min \{ I(t_k, c) + \mathcal{D}(c_{k-1}, c) \mid c \in \mathcal{P} \}.$$

Concerning stability and energy balance we have the following result which relies on the triangle inequality

$$D(e_i, e_k) \leq D(e_i, e_j) + D(e_j, e_k) \quad \text{for all } i, j, k \in \{1, \dots, n\}. \quad (3.1)$$

Theorem 3.1. *Assume that D satisfy the triangle inequality, then the solutions c_k of (IP) are stable and satisfy the discretized energy inequality*

$$\begin{aligned} & \langle \mathbf{G}(t_k) - \mathbf{G}(t_{k+1}), \mathbf{U}(t_{k+1}, c_{k+1}) \rangle \\ & \leq I(t_{k+1}, c_{k+1}) + \mathcal{D}(c_k, c_{k+1}) - I(t_k, c_k) \leq \langle \mathbf{G}(t_k) - \mathbf{G}(t_{k+1}), \mathbf{U}(t_k, c_k) \rangle. \end{aligned}$$

Proof. For all $a \in \mathcal{P}$ we have

$$\begin{aligned} I(t_k, a) + \mathcal{D}(c_k, a) &= (I(t_k, a) + \mathcal{D}(c_{k-1}, a)) + \mathcal{D}(c_k, a) - \mathcal{D}(c_{k-1}, a) \\ &\geq (I(t_k, c_k) + \mathcal{D}(c_{k-1}, c_k) + \mathcal{D}(c_k, a)) - \mathcal{D}(c_{k-1}, a) \geq I(t_k, c_k), \end{aligned}$$

where the infimum property in (IP) was used in the first estimate and the triangle inequality in the second. This proves stability.

The first estimate follows since c_k is stable, in particular with respect to c_{k+1} :

$$\begin{aligned} I(t_{k+1}, c_{k+1}) + \mathcal{D}(c_k, c_{k+1}) &= I(t_k, c_{k+1}) + \mathcal{D}(c_k, c_{k+1}) + [I(t_{k+1}, c_{k+1}) - I(t_k, c_{k+1})] \\ &\geq I(t_k, c_k) + [I(t_{k+1}, c_{k+1}) - E(t_k, c_{k+1}, \mathbf{U}(t_k, c_{k+1}))] \\ &\geq I(t_k, c_k) + [I(t_{k+1}, c_{k+1}) - E(t_k, c_{k+1}, \mathbf{U}(t_{k+1}, c_{k+1}))] \\ &= I(t_k, c_k) + \langle \mathbf{G}(t_k) - \mathbf{G}(t_{k+1}), \mathbf{U}(t_{k+1}, c_{k+1}) \rangle. \end{aligned}$$

The second estimate in the energy inequality follows from the minimizing properties of c_{k+1} :

$$\begin{aligned} I(t_{k+1}, c_{k+1}) + \mathcal{D}(c_k, c_{k+1}) &\leq I(t_{k+1}, c_k) = E(t_{k+1}, c_k, \mathbf{U}(t_{k+1}, c_k)) \\ &\leq E(t_{k+1}, c_k, \mathbf{U}(t_k, c_k)) = I(t_k, c_k) - \langle \mathbf{G}(t_{k+1}) - \mathbf{G}(t_k), \mathbf{U}(t_k, c_k) \rangle. \end{aligned}$$

□

The main problem in treating (IP) as a mathematical or numerical problem is that in general this minimization process does not have a solution. For given c_{k-1} the infimum α_k of $J(t_k, c_{k-1}, c_k) = I(t_k, c_k) + \mathcal{D}(c_{k-1}, c_k)$ with respect to c_k is not attained. This means that we can find c_k^ε with $J_k(c_{k-1}, c_k^\varepsilon) \leq \varepsilon + \alpha_k$ for each $\varepsilon > 0$ but not for $\varepsilon = 0$. This problem arises from the physical fact that the sequence c_k^ε has to develop finer and finer structure such that the sequence c_k^ε does not converge pointwise in Ω .

4 Relaxation

For every minimizing sequence $(c_k^\varepsilon)_{\varepsilon \rightarrow 0}$ there exist subsequences which converge in a weak* to a function \widehat{c}_k . Here weak* convergence $c^\varepsilon \xrightarrow{*} \widehat{c}$ means that for all $f \in C(\overline{\Omega})$ we have $\int_{\Omega} c^\varepsilon(\mathbf{x}) \cdot f(\mathbf{x}) \, d\mathbf{x} \rightarrow \int_{\Omega} \widehat{c}(\mathbf{x}) \cdot f(\mathbf{x}) \, d\mathbf{x}$ as $\varepsilon \rightarrow 0$. A more physical interpretation of weak* convergence is that for almost all $\mathbf{x} \in \Omega$ and all $r > 0$ we have

$$\int_{|\mathbf{y}-\mathbf{x}|<r} c^\varepsilon(\mathbf{y}) \, d\mathbf{y} \rightarrow \int_{|\mathbf{y}-\mathbf{x}|<r} \widehat{c}(\mathbf{y}) \, d\mathbf{y} \quad \text{for } \varepsilon \rightarrow 0.$$

Here r defines a mesoscopic scale while c^ε has spatial oscillations on microscopic scales. The limit function \widehat{c} defines mesoscopically averaged phase mixtures and takes no longer take values in P but its convex hull

$$\widehat{P} = \text{conv}(P) = \left\{ \widehat{c} \in \mathbb{R}^n \mid \widehat{c} = \sum_{j=1}^n \theta_j e_j, \theta_j \geq 0, \sum_{j=1}^n \theta_j = 1 \right\}.$$

We also set $\widehat{\mathcal{P}} = \{ \widehat{c} : \Omega \rightarrow \widehat{P} \mid \widehat{c} \text{ measurable} \}$. Then $\widehat{\mathcal{P}}$ is the closure of $\text{conv}(\mathcal{P})$ with respect to the strong $L^1(\Omega)$ topology and also the weak* closure of \mathcal{P} .

Thus, we are automatically led to consider microscopically fine phase mixtures $c_k^\varepsilon \in \mathcal{P}$, $\varepsilon \ll 1$ which can be described by mesoscopical functions $\widehat{c} \in \widehat{\mathcal{P}}$ which contain information on the volume fractions $\theta_j(\mathbf{x}) \stackrel{\text{def}}{=} \widehat{c}(\mathbf{x}) \cdot e_j$ of the phase e_j in an infinitesimal neighborhood of $\mathbf{x} \in \Omega$.

Since many physically interesting quantities only depend on the limit \widehat{c}_k it is desirable to find \widehat{c}_k directly through a new incremental problem. The mathematical tool to be used here is the method of relaxation (see [Rou97]) which is well-known in the theory of non-convex variational problems like in optimal design theory.

We note here that there is a rich literature on relaxation of one functional. However, there seem to be no result for incremental problems. The new difficulty is that the minimizing sequences between the different incremental levels are not independent. In relaxation often one only uses the weak* limit and not more general informations on the oscillations of the minimizing sequences. Thus, it is not clear how to recover all the needed informations. Here we proceed by suggesting a mathematical way of relaxation. Thus, we take into account that this relaxation is useful only in certain situations, see Section 6 for a further discussion.

The relaxation of the functional $J_k(a, c) = I(t_k, c) + \mathcal{D}(a, c)$, $a, c \in \mathcal{P}$, is defined via

$$\widehat{J}_k(\widehat{a}, \widehat{c}) = \inf \left\{ \liminf_{\varepsilon \rightarrow 0} J_k(a^\varepsilon, c^\varepsilon) \mid a^\varepsilon, c^\varepsilon \in \mathcal{P}, a^\varepsilon \xrightarrow{*} \widehat{a}, c^\varepsilon \xrightarrow{*} \widehat{c} \right\}, \quad (4.1)$$

and leads to the **relaxed incremental problem**

(RIP) For given $c_0 \in \mathcal{P}$ find $\widehat{c}_1, \dots, \widehat{c}_n \in \widehat{\mathcal{P}}$ such that $\widehat{c}_k = \arg \min \widehat{J}_k(\widehat{c}_{k-1}, \cdot)$.

Here, $J_k : \widehat{\mathcal{P}}^2 \rightarrow \mathbb{R}$ is weak* lower-semicontinuous, which implies that the infimum of $\widehat{J}_k(\widehat{c}_{k-1}, \widehat{c}_k)$ over $\widehat{c}_k \in \widehat{\mathcal{P}}$ is attained. To solve (RIP) we have to find a more explicit form of \widehat{J}_k . In fact, due to the special dependences of $I(t_k, c)$ and $\mathcal{D}(a, c)$ on $a, c \in \mathcal{P}$ one can find it explicitly with the help of the **mixture function** $\widehat{W}_{\widehat{c}}(\varepsilon)$. It is defined as follows:

$$\widehat{W}_{\widehat{c}}(\varepsilon_0) \stackrel{\text{def}}{=} \inf \left\{ \int_{(0,1)^d} W_{c(\mathbf{y})}(\varepsilon_0 + \varepsilon(\phi)(\mathbf{y})) \, d\mathbf{y} \mid \phi \in H_0^1((0,1)^d), c \in \mathcal{P}, \int_{(0,1)^d} c(\mathbf{y}) \, d\mathbf{y} = \widehat{c} \right\}.$$

This function describes the deformation energy of mixtures, it is not postulated but follows from an exact mathematical theory which is similar to homogenization theory. In fact there is a big literature on methods to how to calculate or estimate $\widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon})$ which relates to optimal bounds for composite materials with given volume fractions, see [Koh91, Bha93, ShW98].

The following theorem which is proved in [The99] (see also [MTL98]) states that the relaxation \widehat{J}_k can be found by relaxing $I(t_k, \cdot)$ and $\mathcal{D}(\cdot, \cdot)$ separately. Intuitively this follows since only the Gibbs' functional I imposes conditions on the micro-structure of c_k^ε while the dissipation functional \mathcal{D} sees just the volume fractions. However, we recall that this nice result is only valid since we made the modeling assumption that the relaxation of the incremental problem is given through the joint relaxation \widehat{J}_k in (4.1).

Theorem 4.1. *We have $J_k(\widehat{a}, \widehat{c}) = \widehat{I}(t_k, \widehat{c}) + \widehat{D}(\widehat{a}, \widehat{c})$, where*

$$\widehat{I}(t, \widehat{c}) = \inf \{ \widehat{E}(t, \widehat{c}, \mathbf{u}) \mid \mathbf{u} \in V(t) \} \quad \text{and} \quad \widehat{D}(\widehat{a}, \widehat{c}) = \int_{\Omega} \widehat{D}(\widehat{a}(\mathbf{x}), \widehat{c}(\mathbf{x})) \, d\mathbf{x}$$

$$\text{with } \widehat{E}(t, \widehat{c}, \mathbf{u}) = \int_{\Omega} \widehat{W}_{\widehat{c}(\mathbf{x})}(\boldsymbol{\varepsilon}(\mathbf{u})(\mathbf{x})) \, d\mathbf{x} - \langle \mathbf{G}(t), \mathbf{u} \rangle$$

$$\text{and } \widehat{D}(\widehat{a}, \widehat{c}) = \min \left\{ \sum_{j=1}^{2n} \lambda_j D(a_j, c_j) \mid \lambda_j > 0, a_j, c_j \in P, (\widehat{a}, \widehat{c}) = \sum_{j=1}^{2n} \lambda_j (a_j, c_j) \right\}.$$

This shows that the relaxed incremental problem is still of the same type as the original incremental problem. However, it was essential to enlarge the function space from pure phase functions $c \in \mathcal{P}$ to phase mixtures $\widehat{c} \in \widehat{\mathcal{P}}$ in order to obtain existence of solutions.

Under the natural assumption that D satisfies the triangle inequality (3.1) it is possible to prove that \widehat{D} has the form $\widehat{D}(\widehat{a}, \widehat{c}) = \Delta(\widehat{a} - \widehat{c})$ with a convex function $\Delta : \mathbb{R}^n \rightarrow [0, \infty)$ which is homogeneous of degree 1.

5 The mixture function

A major problem in applications is to calculate the mixture function under given elasticity tensors \mathbb{E}_i and transformation strains \mathbf{d}_i in (2.1). The following general results are provided in [MTL98, Mie99].

Theorem 5.1. (a) *For fixed $\boldsymbol{\varepsilon}$, the function $\widehat{c} \mapsto \widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon})$ is convex on \widehat{P} .*

(b) *For fixed \widehat{c} , the function $\mathbf{F} \mapsto \widehat{W}_{\widehat{c}}(\frac{1}{2}(\mathbf{F} + \mathbf{F}^T))$ is quasi-convex on $\mathbb{R}^{d \times d}$.*

(c) *For continuous $\widehat{m} : \widehat{P} \rightarrow \mathbb{R}$ define $\widehat{\Psi}(\boldsymbol{\varepsilon}) = \min \{ \widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon}) + \widehat{m}(\widehat{c}) \mid \widehat{c} \in \widehat{P} \}$. Then, for convex $\widehat{m} : \widehat{P} \rightarrow \mathbb{R}$ the function $\mathbf{F} \mapsto \widehat{\Psi}(\frac{1}{2}(\mathbf{F} + \mathbf{F}^T))$ is quasi-convex.*

(d) *If \mathcal{L} denotes the Legendre transform on $\mathbb{R}_{\text{sym}}^{d \times d}$ then we have*

$$\mathcal{L} \left(\sum_{j=1}^n \theta_j \mathcal{L} W_{e_j}(\cdot) \right) (\boldsymbol{\varepsilon}) \leq \widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon}) \leq \sum_{j=1}^n \theta_j W_{e_j}(\boldsymbol{\varepsilon}) \quad \text{where } \theta_j = \widehat{c} \cdot e_j.$$

Unfortunately an explicit evaluation of the mixture function is only possible in simple situations. In space dimension $d = 1$ it is not difficult to show (see [Mie99]) that

$$\begin{aligned} \widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon}) &= \frac{1}{2} \widehat{\mathbb{E}}(\widehat{c})(\boldsymbol{\varepsilon} - \widehat{\mathbf{d}}(\widehat{c}))^2 + \widehat{\beta}(\widehat{c}), \quad \text{with} \\ \widehat{\mathbb{E}}(\widehat{c}) &= 1 / (\sum_1^n \theta_j \mathbb{E}_j), \quad \widehat{\mathbf{d}}(\widehat{c}) = \sum_1^n \theta_j \mathbf{d}_j \quad \text{and} \quad \widehat{\beta}(\widehat{c}) = \sum_1^n \theta_j \beta_j. \end{aligned}$$

Up to now, for higher dimension only the case of phases with identical elasticity tensors is tractable. With $\mathbb{E} = \mathbb{E}_j$ for $j = 1, \dots, n$ we obtain

$$\widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \widehat{\mathbf{d}}(\widehat{c})) : \mathbb{E}(\boldsymbol{\varepsilon} - \widehat{\mathbf{d}}(\widehat{c})) + \sum_1^n \theta_j \beta_j + B(\widehat{c}),$$

where $\widehat{\mathbf{d}}(\widehat{c}) = \sum_1^n \theta_j \mathbf{d}_j$ and the mixture energy $B(\widehat{c})$ takes the form

$$B(\widehat{c}) = \inf \left\{ \frac{1}{2} \int_{(0,1)^d} (\widehat{\mathbf{d}}(c(\mathbf{x}) - \widehat{c}) - \boldsymbol{\varepsilon}(\mathbf{v})(\mathbf{x})) : \mathbb{E}(\widehat{\mathbf{d}}(c(\mathbf{x}) - \widehat{c}) - \boldsymbol{\varepsilon}(\mathbf{v})(\mathbf{x})) \, d\mathbf{x} \mid c \in \mathcal{P}, \int_{(0,1)^d} c(\mathbf{x}) \, d\mathbf{x} = \widehat{c}, \mathbf{v} \in H_0^1((0,1)^d) \right\}.$$

This shows that B is always nonnegative, however, it can be 0 even so the integrals in the infimum are all positive. The case of two phases was studied completely in [Koh91], and with $\widehat{c}_\theta = \theta e_1 + (1-\theta)e_2$ for $\theta \in [0, 1]$ we have

$$B(\widehat{c}_\theta) = \frac{1}{2}\theta(1-\theta)[(\mathbf{d}_1 - \mathbf{d}_2) : \mathbb{E}(\mathbf{d}_1 - \mathbf{d}_2) - b] \quad (5.1)$$

with $b = \max \left\{ \frac{[(\mathbf{d}_1 - \mathbf{d}_2) : \mathbb{E}\mathbf{S}]^2}{\mathbf{S} : \mathbb{E}\mathbf{S}} \mid \mathbf{S} = \boldsymbol{\xi} \otimes \mathbf{v} + \mathbf{v} \otimes \boldsymbol{\xi}, \boldsymbol{\xi}, \mathbf{v} \in \mathbb{R}^d \setminus \{0\} \right\}.$

Thus, for two phases we have the well-known quadratic mixture contribution which is widely used in the engineering literature, see e.g. [Lev97, KL*97, KuM98]. However, it can be shown (see [Koh91, MTL98]) that for more than 2 phases the function B is no longer differentiable. Using the methods in [ShW98] it is possible to find either exact expressions or at least nontrivial lower bounds for $B(\widehat{c})$ for cases with $n \geq 3$.

6 The approximate incremental problem

As mentioned above, the relaxation of incremental problems is not yet understood. It is by no means clear that it is useful to relax the functional $J_k(a, c) = I(t_k, c) + \mathcal{D}(a, c)$ simultaneous in both variables. To decide what kind of relaxation is appropriate we have to ask whether it gives solutions which are close to solutions which are observed in experiments. Clearly in experiments there is never arbitrarily fine micro-structure. Thus, solutions remain in quasi-optimal states due to some microscopical effects which are not accounted for in our model. One such feature is interfacial energy at the boundaries between the different domains of the phases. Here we just mention one way how relaxations can be justified which involves the **approximate incremental problem**.

(AIP) $_\varepsilon$: Given c_0 find $c_j^\varepsilon \in \mathcal{P}$ such that

$$I(t_k, c_k^\varepsilon) + \mathcal{D}(c_{k-1}^\varepsilon, c_k^\varepsilon) \leq \varepsilon + \inf \left\{ I(t_k, c) + \mathcal{D}(c_{k-1}^\varepsilon, c) \mid c \in \mathcal{P} \right\}.$$

By definition of the infimum it is trivial, that (AIP) $_\varepsilon$ has for all $\varepsilon > 0$ solutions. For $\varepsilon \rightarrow 0$ subsequences of these solutions converge weak* to limits \widehat{c}_k . A suitable relaxation $\widehat{J}_k(\cdot, \cdot)$ now should satisfy at least one of the following two conditions.

(Q1) If the sequences (c_k^ε) of solutions of (AIP) $_\varepsilon$ have weak* limits $\widehat{c}_k \in \widehat{\mathcal{P}}$, then these limits solve (RIP).

(Q2) If (\widehat{c}_k) solves (RIP) then there exist solutions (c_k^ε) of $(\text{AIP})_\varepsilon$ such that $c_k^\varepsilon \xrightarrow{*} \widehat{c}_k$ for $\varepsilon \rightarrow 0$.

Under the rather restrictive assumption that we have only two phases with the same elasticity tensor it is shown in [The99] that the relaxation given above satisfies the condition (Q2), however the status of (Q1) remains open.

For more general situations like more phases, different elasticity tensors or for nonlinear elasticity theory there seem to be little hope that the simple relaxation in (4.1) remains good enough. We rather expect that more information is needed to characterize the micro-structures. At the moment we only control the volume averages. However, in more general situations it might be necessary to control also the way micro-structures are formed, e.g., by the H-measure or by more general objects.

7 Reduction for (RIP)

Each step in the relaxed incremental problem consists in a minimization of $\widehat{I}(t_k, \cdot) + \widehat{D}(\widehat{c}_{k-1}, \cdot)$ over $\widehat{\mathcal{P}}$. The functional $\widehat{I}(t, \widehat{c})$ is itself defined as the infimum of $\widehat{E}(t, \widehat{c}, v)$ over all admissible deformations. Thus, we have

$$(\widehat{c}_k, \mathbf{u}_k) = \arg \min \{ \widehat{E}(t_k, \widehat{c}, \mathbf{v}) + \widehat{D}(\widehat{c}_{k-1}, \widehat{c}) \mid \widehat{c} \in \widehat{\mathcal{P}}, \mathbf{v} \in V(t) \}.$$

From the explicit form of \widehat{E} and \widehat{D} we see that the unknown \widehat{c}_k occurs under both integral only pointwise without any derivatives involved.

Defining the functions

$$\begin{aligned} \widehat{\Psi}(\widehat{a}, \boldsymbol{\varepsilon}) &= \min \{ \widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon}) + \widehat{D}(\widehat{a}, \widehat{c}) \mid \widehat{c} \in \widehat{\mathcal{P}} \} \quad \text{and} \\ \widehat{C}(\widehat{a}, \boldsymbol{\varepsilon}) &= \arg \min \{ \widehat{W}_{\widehat{c}}(\boldsymbol{\varepsilon}) + \widehat{D}(\widehat{a}, \widehat{c}) \mid \widehat{c} \in \widehat{\mathcal{P}} \}, \end{aligned}$$

and the functional

$$\widehat{\mathcal{J}}(t, \widehat{a}, \mathbf{u}) = \int_{\Omega} \widehat{\Psi}(\widehat{a}(x), \nabla \mathbf{u}(x)) \, d\mathbf{x} - \langle \mathbf{G}(t), \mathbf{u} \rangle,$$

(RIP) can be reformulated as follows

(RIP)' Given $c_0 \in \mathcal{P}$ find $(\widehat{c}_j, \mathbf{u}_j) \in \widehat{\mathcal{P}} \times V(t_j)$, $j = 1, \dots, n$, such that

$$\mathbf{u}_k = \operatorname{armin} \{ \widehat{\mathcal{J}}(t_k, \widehat{c}_{k-1}, v) \mid v \in V(t_k) \} \quad \text{and} \quad \widehat{c}_k(\mathbf{x}) = \widehat{C}(\widehat{c}_{k-1}(\mathbf{x}), \boldsymbol{\varepsilon}(\mathbf{u}_k)(\mathbf{x})).$$

The formulation of (RIP)' has the major advantage that it reduces to a simple variational problem for the variable $\mathbf{u}_k \in V(t)$. From Theorem 5.1(c) it follows that $\mathbf{F} \mapsto \widehat{\Psi}(\widehat{a}, \frac{1}{2}(\mathbf{F} + \mathbf{F}^T))$ is quasi-convex, hence the existence of a minimizer \mathbf{u}_k is standard. There are two important messages in respect to (RIP)'. First, the function $\widehat{\Psi}(\widehat{a}, \boldsymbol{\varepsilon})$ is in principle completely determined from the energy densities $W_{e_j}(\boldsymbol{\varepsilon})$ and the dissipation coefficients $\kappa_{i \rightarrow j} = D(e_i, e_j)$. Second, the solution of one incremental step reduces to solving one

(nonlinear) elliptic problem, namely that associated to minimizing $\widehat{\mathcal{J}}(t_k, \widehat{c}_{k-1}, \cdot)$. The associated new phase function \widehat{c}_k is obtained by pointwise evaluating \widehat{C} as given in (RIP)'.

The function $\Psi(\widehat{a}, \boldsymbol{\varepsilon})$ is a constitutive function and it can be calculated either analytically or numerically before even starting to solve the incremental problem (RIP). For the above case of two phases with the same elasticity tensor \mathbb{E} and $\kappa = \kappa_{1 \rightarrow 2} = \kappa_{2 \rightarrow 1}$ we obtain

$$\begin{aligned}\widehat{\Psi}(\widehat{c}_\theta, \boldsymbol{\varepsilon}) &= \frac{1}{2}(\boldsymbol{\varepsilon} - \mathbf{d}_2) : \mathbb{E}(\boldsymbol{\varepsilon} - \mathbf{d}_2) + \beta_2 + 2\beta \mathcal{G}_{\kappa/(2b)}(\theta, \boldsymbol{\varepsilon} : \widetilde{\mathbf{d}} + a), \\ \widehat{C}(\widehat{c}_\theta, \boldsymbol{\varepsilon}) &= \vartheta e_1 + (1 - \vartheta)e_2 \quad \text{with } \vartheta = \Theta_{\kappa/(2b)}(\theta, \boldsymbol{\varepsilon} : \widetilde{\mathbf{d}} + a),\end{aligned}$$

with b from (5.1), $a = \frac{1}{4b}(\mathbf{d}_1 : \mathbb{E} \mathbf{d}_1 - \mathbf{d}_2 : \mathbb{E} \mathbf{d}_2 + 2\beta_1 - 2\beta_2) - 1/2$ and $\widetilde{\mathbf{d}} = \frac{1}{2b} \mathbb{E}(\mathbf{d}_2 - \mathbf{d}_1)$. Here we have used the explicit functions

$$\mathcal{G}_\rho(\vartheta, \eta) = \begin{cases} \rho\vartheta & \text{for } \eta \leq -\rho, \\ \rho\vartheta - (\eta + \rho)^2/2 & \text{for } \eta \in [-\rho, \vartheta - \rho], \\ \vartheta^2/2 - \eta\vartheta & \text{for } \eta \in [\vartheta - \rho, \vartheta + \rho], \\ -(\eta - \rho)^2/2 - \rho\vartheta & \text{for } \eta \in [\vartheta + \rho, 1 + \rho], \\ 1/2 - \eta + \rho(1 - \vartheta) & \text{for } \eta \geq 1 + \rho. \end{cases} \quad \text{and } \Theta_\rho(\vartheta, \eta) = -\partial_\eta \mathcal{G}_\rho(\vartheta, \eta).$$

We note that that Θ_ρ is increasing in η which implies that \mathcal{G}_ρ is a concave function in η .

In general the function $\boldsymbol{\varepsilon} \mapsto \widehat{\Psi}(\vartheta, \boldsymbol{\varepsilon})$ is not convex, but only quasi-convex. We show this by reducing the general formula to the special case with $d = 3$, $\beta_1 = \beta_2 = 0$, $\mathbf{d}_2 = 0$, $\mathbf{d}_1 = I$, and $\mathbb{E}\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}$, that is linearized elasticity with Lamé constants $\lambda = 0$ and $\mu = 1/2$. We obtain $b = 1/2$, $a = 1$, and $\widetilde{\mathbf{d}} = -I$ and thus arrive at

$$\widehat{\Psi}(\widehat{c}_\theta, \boldsymbol{\varepsilon}) = \frac{1}{2} \|\boldsymbol{\varepsilon}\|^2 + \mathcal{G}_\kappa(\theta, 1 - \boldsymbol{\varepsilon} : I).$$

By our choice of the transformation strains the PT is purely volumetric and thus the nonlinearity of the problem is only due to the trace $\boldsymbol{\varepsilon} : I$ of $\boldsymbol{\varepsilon}$. Restricting further to $\widehat{c} = \frac{1}{2}(e_1 + e_2)$ and evaluating $\widehat{\Psi}(\widehat{c}_{1/2}, \cdot)$ at $\boldsymbol{\varepsilon}_\tau = \tau I$ we find $\widehat{\Psi}(\widehat{c}_{1/2}, \boldsymbol{\varepsilon}_\tau) = 3\tau^2/2 + \mathcal{G}_\kappa(1/2, 1 - 3\tau)$. Clearly this function is non-convex as we find that the second derivative of $\tau \mapsto \widehat{\Psi}(\widehat{c}_{1/2}, \boldsymbol{\varepsilon}_\tau)$ attains the value -6 for $\tau \in (-\kappa, \frac{1}{2} + \kappa) \cup (\frac{1}{2} - \kappa, 1 + \kappa)$ and the value 3 otherwise.

8 The relaxed time-continuous problem

Finally we want to return to the time-continuous situation. Formally this is very easy, as the incremental problem looks identical to the non-relaxed problem. Thus, we can just return the order of arguments. We define stability of \widehat{c} at time t as

$$\widehat{I}(t, \widehat{c}) \leq \widehat{I}(t, \widehat{a}) + \widehat{\mathcal{D}}(\widehat{c}, \widehat{a}) \quad \text{for all } \widehat{a} \in \widehat{\mathcal{P}}.$$

The relaxed energy balance for a process $\widehat{c} : [0, T] \rightarrow \widehat{\mathcal{P}}$ reads

$$\widehat{I}(t, \widehat{c}(t)) + \widehat{\text{Diss}}(\widehat{c}; s, t) = \widehat{I}(s, \widehat{c}(s)) - \int_s^t \langle \widehat{\mathbf{G}}(\tau), \mathbf{U}(\tau, \widehat{c}(\tau)) \rangle d\tau. \quad (8.1)$$

With these generalizations we formulate the **relaxed time-continuous problem**

(RCP) Given $c_0 \in \mathcal{P}$ find $\widehat{c} : [0, T] \rightarrow \widehat{\mathcal{P}}$ with $\widehat{c}(0) = c_0$ such that $\widehat{c}(t)$ is stable at time t and that the energy inequality holds.

The classical way to obtain solutions of the relaxed time-continuous problem is to study the relaxed incremental problem (RIP) for a sequence of partitions of $[0, T]$ whose fineness tends to 0. The essential feature of the problem is that the total dissipation on the interval $[0, T]$, which can be bounded from above a-priori, allows us to control the oscillations in time of the solutions to the incremental problem. In contrast to this, there is no control on spatial oscillations. Hence, the solutions associated to (RIP) will have a weak* limit for almost all $t \in [0, T]$, and it is the task to show that this limit solves (RCP). It is important to note that Theorem 3.1 holds word by word for the relaxed problem if we replace the quantities by the corresponding ones with $\widehat{\cdot}$.

According to [MTL98] we have the following result.

Theorem 8.1. *Consider a continuously differentiable loading function $\mathbf{G} : [0, T] \rightarrow V_\Gamma^*$ and a sequence of time discretizations $0 = t_0^n < t_1^n < \dots < t_{N(n)}^n = T$ whose fineness $\max_{k=1, \dots, N(n)} |t_k^n - t_{k-1}^n|$ tends to 0 as $n \rightarrow \infty$. Moreover, assume $\kappa_{i \rightarrow j} > 0$ for $i \neq j$ and that \mathcal{D} satisfies (3.1). Let $(c_k^n)_{k=0, \dots, N(n)}$ be the solution of (RIP) and consider the piecewise constant function $\widehat{c}^n(t) = \sum_{i=1}^{N(n)} \chi_{[t_{i-1}^n, t_i^n)}(t) \widehat{c}_i^n$. Then there exists a subsequence (n_j) , functions $I^\infty, \delta^\infty : [0, T] \rightarrow \mathbb{R}$ with δ^∞ monotonously increasing and a process $\widehat{c}^\infty : [0, T] \rightarrow \widehat{\mathcal{P}}$ such that*

- (i) $\widehat{c}^\infty(0) = c_0$ and $\widehat{c}^{n_j}(t) \xrightarrow{*} \widehat{c}^\infty(t)$ for almost every $t \in [0, T]$;
- (ii) $\lim_{j \rightarrow \infty} \widehat{\text{Diss}}(\widehat{c}^{n_j}; s, t) = \delta^\infty(t) - \delta^\infty(s)$ and $\lim_{j \rightarrow \infty} \widehat{I}(t, \widehat{c}^{n_j}(t)) = I^\infty(t)$;
- (iii) $\widehat{\text{Diss}}(\widehat{c}^\infty; s, t) \leq \delta^\infty(t) - \delta^\infty(s)$ and $\widehat{I}(t, \widehat{c}^\infty(t)) \leq I^\infty(t)$;
- (iv) $I^\infty(t) + \delta^\infty(t) - \delta^\infty(s) = I^\infty(s) - \int_s^t \langle \dot{\mathbf{G}}(\tau), \mathbf{U}(\tau, \widehat{c}^\infty(\tau)) \rangle d\tau$.

We note that if we have equalities in (iii) then (iv) gives exactly the desired energy equation (8.1). However, in general we can only prove the weak convergence in (i) and the functionals $\widehat{I}(t, \cdot)$ and $\widehat{\text{Diss}}(\cdot; s, t)$ are only weak* lower semicontinuous but not weak* continuous. For the general situation we can only conclude the weakened energy balance

$$\widehat{I}(t, \widehat{c}^\infty(t)) + \widehat{\text{Diss}}(\widehat{c}^\infty; 0, t) \leq \widehat{I}(0, c_0) - \int_0^t \langle \dot{\mathbf{G}}(\tau), \mathbf{U}(\tau, \widehat{c}^\infty(\tau)) \rangle d\tau.$$

Moreover, the above theorem gives no information on the stability of the limiting process $\widehat{c}^\infty : [0, T] \rightarrow \widehat{\mathcal{P}}$.

Both of these remedies could be overcome if we would be able to show that the convergence $\widehat{c}^{n_j}(t) \xrightarrow{*} \widehat{c}^\infty(t)$ is in fact a strong convergence, let us say in $L^1(\Omega, \widehat{\mathcal{P}})$. The functionals $\widehat{I}(t, \cdot) : \widehat{\mathcal{P}} \rightarrow \mathbb{R}$ and $\widehat{D} : \widehat{\mathcal{P}}^2 \rightarrow \mathbb{R}$ are continuous with respect to the strong L^1 on $\widehat{\mathcal{P}}$ and hence we would obtain the desired properties.

Corollary 8.2. *Under the assumptions of the above theorem assume that we additionally know $\widehat{c}^{n_j}(t) \rightarrow \widehat{c}^\infty(t)$ in $L^1(\Omega)$ for almost all $t \in [0, T]$, then $\widehat{c}^\infty : [0, T] \rightarrow \widehat{\mathcal{P}}$ solves (RCP).*

We remark that we should not expect too much spatial oscillations in the sequences \widehat{c}^{n_j} since we are already dealing with a relaxed problem. Thus, it is conceivable that the solutions \widehat{c}_k^n of the incremental problems lie in fact in a subset of $\widehat{\mathcal{P}}$ which is compact with respect to the strong L^1 topology.

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