Mathematical formulation of quasistatic phase transformations with friction using an extremum principle *

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1 Introduction

The aim of this paper is to present a mathematical approach to the theory of phase transformations (PT) in certain elastic materials, like martensitic PT in shape memory alloys. Our theory takes into account quasistatic dissipation effects which can prevent PT until a certain energetic threshold is reached. This quasistatic dissipation is proportional to the volume of the region where the PT occurs. Thinking in terms of phase boundaries, the dissipation is proportional to the coated volume. This is in analogy to dry friction between rigid or elastic bodies where the coated area is relevant. Thus, a PT is possible whenever the associated gain in the Gibbs' energy of the whole system larger than the energy which is dissipated through the PT. Moreover, we use an *extremum principle* to determine which PT (what phases are created in what regions) out of the set of all possible PT does occur. This principle is formulated in [Lev95, Lev97]) and says that PT occur as soon as they are possible and always those PT actually occurs which minimizes the difference of the dissipation and the gain in the Gibbs' energy. This global version of the extremum principle appears first in [Lev98]. While in these works the theory is presented quite generally including plastic effects as well as surface energies, we here restrict ourselves to the purely elastic case and neglect surface energies between the phase boundaries. This limits the applicability but makes the problem mathematically accessible since the extremum principle reduces in this case to the stability condition for the phase distributions.

Every material point x in the body $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, can be in one of n possible phases e_j, where $P = \{e_1, \ldots, e_n\}$ is the set of all possible phases. The material

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properties of each phase are given by the energy density $W_{e_j}(F)$ where $F = \nabla u$ is the deformation gradient. In martensitic PT one often assumes $W_{e_j}(F) = W(FT_j^{-1}) + \beta_j$ with a fixed energy density W, $T_1 = I$ and $\beta_1 = 0$ for the austenite phase, and $T_j - I$ are the transformation strains for the martensitic phases (e.g. $j = 2, \dots, 13$ for PT from a cubic to a monoclinic lattice). The matrices T_j are typically related to each other by the crystallographic symmetry group, and $\beta_j = \beta$ for $j = 2, \dots, n$ where β is positive (negative) if we are below (above) the critical temperature. The whole analysis works for general inhomogeneous materials with $W_{e_j}(x, F)$ but for notational convenience we restrict ourself to the homogeneous case.

A function $c : \Omega \to P$ is called a state of the system and for each (process) time dependent loading $G(t)$ the Gibbs' energy is given by

$$I(t, c) = \inf\{ \int_\Omega W_{c(x)}(\nabla u(x)) \, \mathrm{d}x - \langle G(t), u \rangle \; : \; u \in V \},$$

where V is the set of kinematically admissible deformations and $\langle \cdot, \cdot \rangle$ denotes the duality pairing between V and its dual space. Under the assumptions that at most one PT occurs at each material point the dissipation of a PT from state $a : \Omega \to P$ into $c : \Omega \to P$ is

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

Here $\kappa_{j \to j} = 0$, and $\kappa_{i \to j} > 0$ for $j \neq i$ are the dissipation coefficients for a PT from e_i into e_j. They serve as a threshold which makes PT more difficult. A family of states $(c(t))_{t \in [0,T]}$ is called a process, and the total amount of dissipation due to PT in the time interval $[t_1, t_2]$ is denoted by $\mathrm{Diss}(c; t_1, t_2)$.

We say that a state c is *stable at time t* if

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

This stability means exactly that there is no admissable PT from the given state $c(t)$ which has a gain in the Gibbs' energy which is larger than the associated dissipation. With this notion we give the following time–continuous formulation of the extremum principle.

> **(CP)** *For given c_0 find a process $c : [0, T] \times \Omega \to P$ with $c(0, x) = c_0(x)$ such that for all t_1, t_2 with $0 \leq t_1 \leq t_2 \leq T$ we have $I(t_2, c(t_2)) \leq I(t_1, c(t_1)) - \mathrm{Diss}(c; t_1, t_2) - \int_{t_1}^{t_2} \langle \dot{G}(s), u(s) \rangle \, \mathrm{d}s$ and $c(t_1)$ is stable at t_1.*

The first condition is the energy inequality for the whole body which includes as last term the work of the external forces. We might as well have imposed energy equality, but due to the relaxation process done below we would have to give up such an equality anyway. The importance of the dissipation by friction is that it is defined quasistatically and it is always nonnegative. Hence, it gives to hysteretic behavior as observed in experiments.

In general we cannot expect to find solutions of (CP) since it is not even clear whether for a given loading $G(t)$ there is any stable state $c : \Omega \to P$. A natural way to find stable states at time t is to minimize $I(t, c)$ over all c. Clearly such a minimizer must be stable, however, in general we can only expect to find a minimizing sequence c_n, that is $I(t, c_n) \to \alpha = \inf\{ I(t, \tilde{c}) \; : \; \tilde{c} : \Omega \to P \}$. The weak limit $\hat{c}$ of the sequence c_n will no longer be a simple phase function but gives rise to infinitesimally fine phase mixtures. The goal of this work is to discuss rigorous extensions of the problem from classical states c

with $c(t,x) \in P$ to phase mixtures $\widehat{c}$ with $\widehat{c}(t,x) \in \widehat{P} = \mathrm{conv}(P)$. In mathematical terms such our procedure is called a relaxation. We insist however, that we do not include new modeling assumptions into a mixture theory, but we want to see how far the given functions $W_{e_j}(F)$ can be used to derive a consistent mixture theory.

At this point we want to connect our theory to the purely static theory of PT without dissipation which an active mathematical subject, see [BaJ87, BaJ92] and the survey [Mül98]. For our mechanical situation it would mean to consider only one stored energy function

$$\overline{W}(F) = \min\{\, W_{e_j}(F) \ : \ j = 1, \ldots, n \,\},$$

which now is no longer quasiconvex but has potential wells in the sets $\mathrm{SO}(3)T_j$. In minimizing the functional $\overline{E}(t,u) = \int_\Omega \overline{W}(\nabla u(x))\,\mathrm{d}x$. Again the minimum of $\overline{E}(t,\cdot)$ is not achieved but minimizing sequences show the development of microstructure. For a function u we say that the point $x \in \Omega$ is the phase e_j if $\overline{W}(\nabla u(x)) = W_{e_j}(\nabla u(x))$. Of course, when always looking for the global minimizer we cannot obtain hysteretic behavior in any quasistatic loading process as no time direction is prefered. Nevertheless hysteretic behavior can occur (see [BaCJ95]) due to local strong minimizers which have a true potential barrier in the function space. To describe this phenomenon with our approach we have to choose the dissipation functional $\mathcal{D}(a,c)$ such that for each such local strong minimizer u_j the associated phase function $c_j : \Omega \to P$ is a global minimum of $a \mapsto I(t,a) + \mathcal{D}(c_j, a)$.

The main idea to find the proper relaxation is to replace the time-continuous problem (CP) by an incremental problem (IP) which has a variational structure arising from the extremum principle. The variational problem can be relaxed using mathematical tools leading to the relaxed incremental problem (RIP). From this relaxation we can state a time-continuous relaxed problem (RCP). Another successful relaxation of a time-continuous problem for pattern formation in magnetic fluids was obtained in [Ott98]; there again an incremental problem in variational form was formulated whose relaxation appears to be the incremental problem of the time-continuous relaxed problem.

To be specific, for $0 < t_1 < \ldots < t_{N-1} < t_N = T$ 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.*

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 $J_k(c_{k-1}, c_k^\varepsilon) \le \varepsilon + \alpha_k$ 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. However, subsequences will converge in a weak sense to a function $\widehat{c}_k$ which now does no longer take values in P but its convex hull

$$\widehat{P} = \{\, \widehat{c} \in I\!R^n \ : \ \widehat{c} = \textstyle\sum_{j=1}^n \theta_j e_j, \ \theta_j \ge 0, \ \sum_{j=1}^n \theta_j = 1 \,\}.$$

Thus, we are automatically led to consider microscopically fine phase mixtures c_k^ε, $\varepsilon \ll 1$ which can be described by macroscopical functions $\widehat{c}(x)$ which contain only information on the volume fractions $\theta_j(x)$ of the phases.

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 [Dac89, Rou97]) which is well–known in the theory of nonconvex variational problems like in optimal design theory. There the aim is to find an extension $\widehat{J}_k(\widehat{a},\widehat{c})$ of $J_k(a,c)$ to functions $\widehat{a},\widehat{c}:\Omega\to\widehat{P}$ such the solutions $\widehat{c}_1,\dots,\widehat{c}_N$ of the following *relaxed incremental problem* (RIP) are in fact the weak limits of minimizing sequences c_k^ε for (IP). The question of the proper relaxation for such incremental problems is not yet understood, since in general it is not enough to consider the relaxation of $J(t_k,\cdot,\cdot)$, see Question 1 and 2 at the end of Section 4.2 and [The98] for positive and negative results in this direction.

According to [The98] the relaxation of $J(t_k,\cdot,\cdot)$ is obtained by separate relaxation of I and D:

$$\begin{aligned}&\widehat{J}(t_k,\widehat{a},\widehat{c})=\widehat{I}(t_k,\widehat{c})+\widehat{\mathcal{D}}(\widehat{a},\widehat{c}),\ \text{ where}\\ &\widehat{I}(t_k,\widehat{c})=\inf\{\,\widehat{E}(t,\widehat{c},u)\ :\ u\in V\,\}\text{ and }\widehat{\mathcal{D}}(\widehat{a},\widehat{c})=\textstyle\int_\Omega\widehat{D}(\widehat{a}(x),\widehat{c}(x))\,\mathrm{d}x.\end{aligned}$$

Here $\widehat{E}(t,\widehat{c},u)=\int_\Omega\widehat{W}_{\widehat{c}(x)}(\nabla u)\,\mathrm{d}x-\langle G(t_k),u\rangle$, $\widehat{D}:\widehat{P}\times\widehat{P}\to I\!R_\geq$ is the convex envelope of $D:P\times P\to I\!R_\geq$, see Proposition 4.1. The function $\widehat{W}_{\widehat{c}}(F)$ is defined via

$$\widehat{W}_{\widehat{c}}(F)\overset{\text{def}}{=}\inf\{\,⨍_B W_{c(y)}(F{+}\nabla\phi(y))\,\mathrm{d}y\ :\ \phi\in\mathrm{W}_0^{1,p}(B),\ c(x)\in P,\ ⨍_B c(y)\,\mathrm{d}y=\widehat{c}\,\}$$

and will be called the *mixture function* as it describes the deformation energy of mixtures. Note that this mixture function 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 $\widehat{W}_{\widehat{c}}(F)$ which relates to optimal bounds for composite materials with given volume fractions, see [Koh91, GrK95]. The *relaxed incremental problem* now reads

> **(RIP)** *For given $\widehat{c}_{k-1}$ find $\widehat{c}_k$ such that $\widehat{J}(t_k,\widehat{c}_{k-1},\widehat{c}_k)=\widehat{I}(t_k,\widehat{c}_k)+\widehat{\mathcal{D}}(\widehat{c}_{k-1},\widehat{c}_k)$ is minimal.*

The main advantage of (RIP) is that it consists in minimizing the integral $\int_\Omega[\widehat{W}_{\widehat{c}(x)}(\nabla u(x))+\widehat{D}(\widehat{c}_{k-1}(x),\widehat{c}(x))]\,\mathrm{d}x-\langle G(t_k),u\rangle$ with respect to u and $\widehat{c}$. Taking first the infimum with respect to $\widehat{c}(x)$, which can be done pointwise for $x\in\Omega$, we are left with minimizing

$$\begin{aligned}&\widehat{\mathcal{E}}(t_k,\widehat{c}_{k-1},u)=\textstyle\int_\Omega\widehat{\Psi}(\widehat{c}_{k-1}(x),\nabla u(x))\,\mathrm{d}x-\langle G(t),u\rangle\\ &\text{where }\widehat{\Psi}(\widehat{a},F)=\min\{\,\widehat{W}_{\widehat{c}}(F)+\widehat{D}(\widehat{a},\widehat{c})\ :\ \widehat{c}\in\widehat{P}\,\}.\end{aligned}$$

Here again, the function $\widehat{\Psi}$ is uniquely determined from the family W_{e_j} and the dissipation coefficients $D(e_i,e_j)=\kappa_{i\to j}$, see Section 6.3 for an explicit example. Moreover, $\widehat{c}_k(x)$ can be found after the minimizer u_k, namely $c_k(x)\in\arg\min[\widehat{W}_{(\cdot)}(\nabla u_k(x))+\widehat{D}(\widehat{c}_{k-1}(x),\cdot)]$.

The associated time-continuous problem can now be formulated in terms of the relaxed functionals.

> **(RCP)** *For c_0, find $\widehat{c}:[0,T]\times\Omega\to\widehat{P}$ with $\widehat{c}(0,x)=c_0(x)$ such that for all τ,t with $0\le\tau<t\le T$ we have $\widehat{I}(t,\widehat{c}(t))=\widehat{I}(\tau,\widehat{c}(\tau))-\widehat{\mathrm{Diss}}(\widehat{c};\tau,t)-\int_\tau^t\langle\dot{G}(s),u(s)\rangle\,\mathrm{d}s$, and $\widehat{I}(t,\widetilde{a})+\widehat{\mathcal{D}}(\widehat{c}(t),\widehat{a})\ge\widehat{I}(t,\widehat{c}(t))$ for all $\widehat{a}\in\mathrm{L}^\infty(\Omega,\widehat{P})$.*

Quasistatic processes have been successfully approximated in many other areas with solutions to a finite collection of minimization problems. The reader is referred to [HaR95] where the equivalence of the time continuous formulation and incremental problems is proven for elastoplastic flows. The advantage of this approach is that it offers a natural scheme for the generation of numerical approximations to the time continuous process. See [ACZ, CHM98] for a more general incremental formulation in elastoplasticity, including the case of finite deformations, which again has the form of a minimisation problem, where the appropriate functional has to be minimized with respect to the deformation as well as the internal plastic variables.

In Section 2 the modeling is described in more detail. In Section 3 we treat a very simple one–dimensional model which allows us to compare the time-continuous problem and the incremental problem. In Section 4 we discuss the questions associated to relaxation. In Section 5 we finally consider stability questions of states which are in one phase. This yields criteria for the onset of nucleation as well as the propagation of phase boundaries. The analysis is terminated by explicit calculation of the the relaxed functions like $\widehat{\Psi}(\hat{a}, F)$ in the case of linearized elasticity theory and two phases in Section 6.

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2 Description of the model

We consider an elastic material occupying the domain $\Omega \subset I\!R^d$ in its reference configuration. At each point $x \in \Omega$ the material can be n different phases, denoted by the points $e_j \in I\!R^n$, where e_j is the jth unit vector. We let $P = \{e_1, e_2, \dots, e_n\}$ to denote the set of possible phases. (This special choice of e_j to denote the different phases allows us later on to realize phase mixtures via convex combinations $c \in \widehat{P} = \mathrm{conv}(P)$.)

The elastic material properties are given via the stored energy density $W_{e_j}(x, F)$ where F the deformation gradient ∇u. For given $c \in \mathrm{L}^\infty(\Omega, P)$ and $u \in \mathrm{W}^{1,p}(\Omega)$ the bulk energy or elastic energy is given by

$$E_e(c, u) = \int_\Omega W_{c(x)}(x, \nabla u(x))\, \mathrm{d}x.$$

Throughout this work the energy–density functions W_{e_i} will be written without x–dependency. This should not deceive the reader that the analysis presented in this work is only applicable in the case of single crystals. In fact the focus of our interest is the modeling of poly crystals where every step can also be carried through. Then the energy densities have the form $W_{e_i}(x, F) = \widetilde{W}_{e_i}(R^T(x) F R(x))$, where R is a rotation valued mapping from Ω into the set of matrices, $R(x) = \sum_i \chi_{\omega_i}(x) \cdot R_i$ and (ω_i) is a partition of Ω. Every ω_i corresponds to a grain of the body Ω, by χ_{ω_i} the characteristic function of ω_i is denoted and R_i is the rotation giving the crystalline orientation relative to a fixed reference crystal. The function $x \mapsto R(x)$ is discontinuous at the grain boundaries, so it implicitly determines the shape of each grain as well as its orientation.

Our aim is to describe time-dependent processes which are driven by external forces and boundary conditions. The boundary conditions are imposed by a closed subspace V of $\mathrm{W}^{1,p}(\Omega)$, and the (dead) loading is given as a linear functional $G(t) \in V^*$. To think about something particular, we may consider a subset $\Gamma \subset \partial\Omega$ and let

$$V = \{\, u \in \mathrm{W}^{1,p}(\Omega) \,:\, u = \psi \text{ on } \partial\Omega\setminus\Gamma \,\}, \quad \langle G(t), u\rangle = \int_\Omega f \cdot u \,\mathrm{d}x + \int_\Gamma g \cdot u \,\mathrm{d}\mathcal{H}^{d-1}(x) \quad (2.1)$$

with $f \in \mathrm{L}^\infty(\Omega)$, and $g \in \mathrm{L}^\infty(\Gamma)$. Thus, at time t the system is described by $(c, u) \in \mathrm{L}^\infty(\Omega, P) \times V$ and has the total energy (Gibbs' energy)

$$E(t, c, u) = \int_\Omega W_{c(x)}(\nabla u(x))\, dx - \langle G(t), u\rangle.$$

Here $\langle \cdot, \cdot\rangle$ is the duality pairing in $V^* \times V$.

The process is assumed to be quasistatic which is reminiscent to the fact that u is at each time in elastic equilibrium, in particular we may assume that $u(t) \in V$ is the global minimizer of the total energy for given $c(t)$, that is

$$E(t, c(t), u(t)) = \inf_{v\in V} E(t, c(t), v)\,. \quad (2.2)$$

Throughout this work we will assume that for given (G, c) always a unique minimizer $u = \mathcal{U}(G, c)$ exists. Hence, u is not really needed to describe the process, as it can be recovered from (G, c). Thus, we may define the energy as a function of (t, c) alone, viz.

$$I(t, c) = E(t, c, \mathcal{U}(G, c)) = \inf\{\, E(t, c, v) \,:\, v \in V \,\}.$$

The class of stored energy density functions W_{e_i} admitted in our model is far too large as one could expect many useful results for it. An important subclass for applications are quadratic energy density functions for which $\mathcal{U}(G, c)$ can be found. This approach entails of course the known weakness, that large deformations are not described correctly. Most results for quadratic energies which are important for this model are restricted to the case of two phases and constant coefficients. They rely on a work by KOHN [Koh91], for an exposition in connection with our model see Section 6.

For nonquadratic energy densities only existence of energy minimizing deformations is known, this suffices for the abstract formulation of the time discretized approximation scheme. Most questions which are beyond existence of time discrete solutions are open. The reason we formulate the model in such a great generality is that the abstraction clarifies the structure of the algorithm and the arising problems.

The main ingredient to our theory of phase transformations (PT) is that a PT can only occur when a certain energetic threshold is reached. Each PT dissipates an amount of energy which is proportional to the volume of the region occupied by the transformed material times the constant $\kappa_{i\to j} \geq 0$ depending only the state e_i before and the state e_j after PT. Clearly we have $\kappa_{i\to i} = 0$ and $\kappa_{i\to j} > 0$ for $i \neq j$.

Thus, assuming that the function $c(t, x)$ is such that in the time interval $[t_1, t_2]$ the function $c(\cdot, x)$ changes at most once (that is, at most one PT takes place in each $x \in \Omega$) then the total dissipation is given by

$$\mathcal{D}(c(t_1), c(t_2)) = \int_\Omega D(c(t_1, x), c(t_2, x))\,\mathrm{d}x$$

where D is the function $D : P \times P \to \mathbb{R}_{\geq}; (e_i, e_j) \mapsto \kappa_{i\to j}$.

The restriction of our Ansatz is manifested by the predicted shape of the hysteresis loop. It is too simple to give good a qualitative description of the manifold experimental results for single crystals. However we expect that the averaging process of polycrystals is robust enough to give a reasonable agreement with the predictions from our model. The mesoscopic homogenization which is necessary to compare our model with polycrystals, which are used in applications, is beyond the scope of this work. This question could possibly be investigated by numerical experiments.

To motivate the incremental problems to be defined below we first consider processes with continuous time.

2.1 Continuous time

Using that $u(t,\cdot)$ is in elastic equilibrium, the energy inequality reduces to the relation

$$I(t_2, c(t_2)) + \mathrm{Diss}(c; t_1, t_2) \leq I(t_1, c(t_1)) - \int_{t_1}^{t_2} \langle \dot{G}(t), u(t) \rangle \, \mathrm{d}t, \tag{2.3}$$

where the last term contains the energy contribution of the work done by the external loading. The term $\mathrm{Diss}(c; t_1, t_2)$ includes the dissipation which occurs through phase transformations in the time interval $[t_1, t_2]$. If at some material point several phase transformations occur in this time interval then

$$\mathrm{Diss}(c; t_1, t_2) = \sum_{k=1}^{m} \mathcal{D}(c(s_k), c(s_{k-1})) \quad \text{with } s_k = t_1 + k(t_2 - t_1)/m \tag{2.4}$$

for m sufficiently large. If c represents a smooth process, then of course $\mathrm{Diss}(c; t_1, t_2) = \int_{t_1}^{t_2} \widetilde{D}(c(t))[\dot{c}(t)] \, \mathrm{d}t$, where $\widetilde{D}(c(t))[\dot{c}(t)] = \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Diss}(c; 0, t)$. The integral notation leads to difficulties when general processes with possibly discontinuous c are considered, therefore we will not use it.

The extremum principle from [Lev95] (see Eqn. (198) for the purely elastic case) which says that PT occurs as soon as they are possible, which means that there has to be an associated gain in the Gibbs' energy to be compatible with (2.3). Moreover, from all possibilities of PT those are preferred which maximize the difference between the dissipation and the gain in the Gibbs' energy. We suggest here a possible mathematical formulation of this extremum principle in the case of a continuous process time $t \in [0, T]$. However, at present it is not clear how useful these definitions are since we are only able to deduce partial existence and no uniqueness results from them. We give the following definitions only for completeness and analogy to the time–discrete case, the latter being the main interest of this work.

A phase transformation from c_- to c_+ is possible if the gain in the Gibbs' energy is larger than the dissipation through the interface friction:

$$\mathcal{D}(c_-, c_+) - (I(t, c_-) - I(t, c_+)) \geq 0.$$

The postulate of realizability says that PT occurs as soon as possible which means that for a time–continuous process strict inequality can never occur since otherwise a PT would have occured earlier.

Definition 2.1
A process $c : [0, T] \to L^\infty(\Omega, P)$ is **stable** *if for every $t \in [0, T]$*

$$I(t, a) + \mathcal{D}(c(t), a) \geq I(t, c(t)) \quad \textit{for all } a \in \mathrm{L}^\infty(\Omega, P).$$

The process c satisfies the **strong energy inequality** *if for all $0 \leq t_1 \leq t_2 \leq T$*

$$I(t_2, c(t_2)) + \mathrm{Diss}(c; t_1, t_2) \leq I(t_1, c(t_1)) - \int_{t_1}^{t_2} \langle \dot{G}(t), u(t) \rangle \, \mathrm{d}t.$$

We say that c satisfies the **weak energy inequality** *if the above inequality holds only for $t_1 = 0$.*

Stable processes which satisfy the strong energy inequality are denoted as **admissible**.

Remark 2.2 The definition of stability gives a time–dependent restriction of the state space, it does not see the dynamics of the process. The stability implies that for no time t_1 the process can be changed on $(t_1, t_2]$ such that the difference between dissipation and energy gain is negative. We will use the terms stability principle and extremum principle synonymously. The strong energy inequality is local in time since it suffices to test the inequality in a small interval around every time t. The weak energy inequality is nonlocal in time.

The stability condition is posed globally over the whole body Ω, however it involves all possible variations of the state a. Hence, it is possible to derive local conditions for material points $x \in \Omega$. This is done in Section 5 where we obtain the following two results. The first one can be interpreted as the stability condition of a pure phase e_i with respect to formation of a nucleus including different phases $\widehat{c}$.

Theorem 2.3
(a) Let $c : \Omega \to P$ be a stable state and let $x_0 \in \Omega$ be such that $c(x)$ and $F(x) = \nabla u(x)$ are continuous in $x = x_0$. Then, with we have

$$W_{c(x_0)}(F(x_0)) \leq \widehat{D}(c(x_0), \widehat{a}) + \widehat{W}_{\widehat{a}}(F(x_0)) \quad \textit{for all } \widehat{a} \in \widehat{P}.$$

Here $\widehat{W}_{\widehat{a}}(F)$ and $\widehat{D}$ are defined in Section 4.
(b) Let $c : \Omega \to P$ be a stable state and let $x_0 \in \Omega$ be a point where c has a smooth phase boundary with normal vector ν. Let $(e^\pm, F^\pm)$ be the left and right limits of $(c(x), F(x))$ which satisfy by strain and stress compatibility $F^+ - F^- = a \otimes \nu$ and $T_0 \stackrel{\text{def}}{=} [\partial_F W_{e^+}(F^+) - \partial_F W_{e^-}(F^-)]\nu = 0$. Then we have

$$-D(e^+, e^-) \leq W_{e^-}(F^-) - W_{e^+}(F^+) + T_0 \cdot ([F^+ - F^-]\nu) \leq D(e^-, e^+).$$

The reason we ask admissible processes to satisfy the energy inequality instead of the **energy identity** is of rather technical nature.

Proposition 2.4
Let c be an admissible process. Then the energy inequality is satisfied with "$=$" instead of "$\leq$".

Proof: The mapping $t \mapsto I(t, c(t))$ is differentiable in the sense of distributions, thus

$$\begin{aligned} & I(t_2, c(t_2)) - I(t_1, c(t_1)) + \mathrm{Diss}(c; t_1, t_2) + \textstyle\int_{t_1}^{t_2} \langle \dot{G}(t), u(t) \rangle \, \mathrm{d}t \\ = & \textstyle\int_{t_1}^{t_2} \Big[\frac{\mathrm{d}}{\mathrm{d}t} \Big\{ \int_\Omega W_{c(t,x)}(\nabla u(t,x)) \, \mathrm{d}x - \langle G(t), u(t) \rangle \Big\} + \langle \dot{G}(t), u(t) \rangle \Big] \, \mathrm{d}t + \mathrm{Diss}(c; t_1, t_2) = J. \end{aligned}$$

Defining $\widetilde{W}(t,x,F) = W(c(t,x),F)$ and using the fact that $t \mapsto \langle G(t), \dot{u}\rangle$ is differentiable in the distributional sense one finds that

$$\begin{aligned} J = \; & \int_{t_1}^{t_2} \int_\Omega \partial_1 \widetilde{W}(t,x,\nabla u(t,x)) \,\mathrm{d}x\,\mathrm{d}t + \mathrm{Diss}(c;t_1,t_2) \\ & + \int_{t_1}^{t_2} \left\{ \int_\Omega \sigma(\nabla u(t,x))[\nabla \dot{u}(t,x)]\,\mathrm{d}x - \langle G(t), \dot{u}(t)\rangle \right\} \mathrm{d}t = J_1 + J_2 + J_3 \end{aligned}$$

where $\sigma(F) = \nabla W(F)$. From the fact that $u(t,x)$ is a minimizer of $E(t,c(t),\cdot)$ it follows that the weak form of the Euler–Lagrange equation is satisfied and thus J_3 vanishes. Setting $\widetilde{\widetilde{W}}(s,t,x) = W(c(s,x), \nabla u(t,x))$ and applying the a priori estimates from the existence proof of minimizers to the purely elastic problem in [Mie98] we can infer that $\widetilde{\widetilde{W}} \in L^\infty([t_1,t_2]\times[t_1,t_2], L^1(\Omega))$ holds. From the measurability of $\widetilde{\widetilde{W}}$ follows that

$$\int_{t_1}^{t_2} \int_\Omega \partial_1 \widetilde{\widetilde{W}}(t,t,x)\,\mathrm{d}x\,\mathrm{d}t \geq \inf_{\mathcal{P}} \sum_{i=0}^{|\mathcal{P}|-2} \int_\Omega \left\{ \widetilde{\widetilde{W}}(t_{i+1},t_i,x) - \widetilde{\widetilde{W}}(t_i,t_i,x) \right\} \mathrm{d}x,$$

where $\mathcal{P}$ is the set of finite partitions of the interval $[t_1,t_2]$. We define a dummy variable $v = \mathrm{argmin}_{u\in V} E(t_i, c(t_{i+1}), u)$. The definiton of $\widetilde{\widetilde{W}}$ implies

$$\begin{aligned} J_1 \geq \; & \inf_{\mathcal{P}} \sum_{i=0}^{|\mathcal{P}|-2} \left\{ \int_\Omega W_{c(t_{i+1})}(\nabla v)\,\mathrm{d}x - \langle G(t_i), v\rangle - \left(\int_\Omega W_{c(t_i)}(\nabla u(t_i))\,\mathrm{d}x - \langle G(t_i), u(t_i)\rangle \right) \right. \\ & \left. + \int_\Omega W_{c(t_{i+1})}(\nabla u(t_i))\,\mathrm{d}x - \langle G(t_i), u(t_i)\rangle - \left(\int_\Omega W_{c(t_{i+1})}(\nabla v)\,\mathrm{d}x - \langle G(t_i), v\rangle \right) \right\} \\ \geq \; & \inf_{\mathcal{P}} \sum_{i=0}^{|\mathcal{P}|-2} \left\{ I(t_i, c(t_{i+1})) - I(t_i, c(t_i)) \right\} \\ \geq \; & \inf_{\mathcal{P}} \sum_{i=0}^{|\mathcal{P}|-2} -\mathcal{D}(c(t_i), c(t_{i+1})) = -\mathrm{Diss}(c; t_1, t_2), \end{aligned}$$

where the definition of $I(t,c)$, the stability of the process c and the definition of $\mathrm{Diss}(c;t_1,t_2)$ have been used for the last three steps. This implies that $J_1 + J_2 + J_3 \geq 0$ and the proof is complete. QED

We are led to the following time-continuous problem.

(CP) Given $c_0 \in \mathrm{L}^\infty(\Omega, P)$ find an admissible process $c : [0,T] \to \mathrm{L}^\infty(\Omega, P)$ with $c(0) = c_0$.

2.2 Discrete time

In the theory of quasistatic processes it is very common to consider the system only at a discrete set of times $0 = t_0 < t_1 < \ldots < t_k < \ldots < t_N = T$. Of course, we cannot expect to recover the exact result of the time–continuous problem, but we hope to find a good approximation if all increments $t_k - t_{k-1}$ are small enough.

We have to approximate the two integrals in the energy inequality (2.3) and then reformulate the maximal dissipation principle. The dissipation integral will be approximated via

$$\mathrm{Diss}(c; t_{k-1}, t_k) \approx \mathcal{D}(c(t_{k-1}), c(t_k)) \tag{2.5}$$

and the work of the external loadings via

$$I(t_{k-1},c_{k-1}) - \int_{t_{k-1}}^{t_k}\langle \dot G(t),u(t)\rangle\,\mathrm{d}t \;\approx\; \begin{aligned}[t] &I(t_{k-1},c_{k-1}) - \langle G(t_k)-G(t_{k-1}),u(t_{k-1})\rangle \\ &= E(t_k,c_{k-1},u_{k-1}). \end{aligned} \tag{2.6}$$

For Lipschitz continuous functions $u:[t_{k-1},t_k]\to V$ and $\dot G:[t_{k-1},t_k]\to V^*$ the error is of order $\mathcal{O}(|t_{k-1}-t_k|^2)$. Neglecting this error as well as the error in (2.5), one finds that the stability principle in Definition 2.1 gives approximatively

$$\begin{aligned} &I(t_k,c_k)+\mathcal{D}(c_{k-1},c_k)-E(t_k,c_{k-1},u_{k-1})\le 0\\ &\le I(t_k,a)+\mathcal{D}(c_{k-1},a)-E(t_k,c_{k-1},u_{k-1}) \end{aligned} \tag{2.7}$$

for all $a\in \mathrm{L}^\infty(\Omega,P)$. As $E(t_k,c_{k-1},u_{k-1})$ is given already when c_k has to be determined we arrive at the the following definition for the time–discrete process.

Definition 2.5
A sequence $c_k\in \mathrm{L}^\infty(\Omega,P)$, $k=0,\dots,N$ of phase functions with associated deformations $u_k=\mathcal{U}(G(t_k),c_k)$ satisfies the **incremental extremum principle** *if*

$$I(t_k,c_k)\le I(t_k,a)+\mathcal{D}(c_k,a)\quad \textit{for all } a\in \mathrm{L}^\infty(\Omega,P). \tag{2.8}$$

Thus, the solution to the incremental problem (IP) is found by successively solving the following minimization problems:

(IP) Given $c_0\in \mathrm{L}^\infty(\Omega,P)$ find $c_1,\dots,c_N\in \mathrm{L}^\infty(\Omega,P)$ such that

$$I(t_k,c_k)+\mathcal{D}(c_{k-1},c_k)=\inf\{\,I(t_k,a)+\mathcal{D}(c_{k-1},a)\;:\;a\in \mathrm{L}^\infty(\Omega,P)\,\}.$$

In general the solutions of (IP) may not satisfy the stability principle which is seen if we consider a problem with three phases as follows. Let $V=\mathrm{W}_0^{1,2}(\Omega)$, $G(t)\equiv 0$, and $W_{e_j}(F)=|F|^2+B_j$ with $B_j=2-j$. This implies that for all c and t we have $u\equiv 0$. Hence, $I(t,c)=\mathrm{vol}(\Omega)(\theta_1+\theta_2)$ for $⨍_\Omega c(x)\,\mathrm{d}x=\sum_1^3\theta_j e_j$. Moreover, $c_0\equiv e_1$ and $\kappa_{1\to2}=\kappa_{2\to3}=\kappa<1$ and $\kappa_{1\to3}=10$. Then, $I(t,c)+\mathcal{D}(c_0,c)=\mathrm{vol}(\Omega)(2\theta_1+(1+\kappa)\theta_2+10\theta_3)$. From (IP) we find the solution $c_1\equiv e_2$, but clearly this c_1 is not extremal since $I(t,c)+\mathcal{D}(c_1,c)=\mathrm{vol}(\Omega)((2+\kappa_{2\to1})\theta_1+\theta_2+\kappa\theta_3)$ attains its minimum at $c\equiv e_3$. In this example the problem arises from the fact that D does not satisfy the triangle inequality

$$D(a,c)\le D(a,b)+D(b,c)\quad\text{for all } a,b,c\in P. \tag{2.9}$$

Lemma 2.6
Assume that $D:P\times P\to I\!R_{\ge}$ satisfies (2.9)*, then the solutions of (IP) satisfy the extremal condition* (2.8)*. Moreover, we have the energy inequality $I(t_k,c_k)+\mathcal{D}(c_{k-1},c_k)\le I(t_k,c_{k-1})$.*

The proof is the following simple estimate. For all $a\in \mathrm{L}^\infty(\Omega,P)$ we have

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

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

There is of course a general problem whether the minimization problem (IP) has a solution at all. Note that we have written *inf* rather than *min* indicating the fact that the infimum of $J_k(c) = I(t_k, c) + \mathcal{D}(c_{k-1}, c)$ might not be attained. In general, there only exist minimizing sequences c^j, that is $J_k(c^j) \to \alpha = \inf\{\, J_k(c) \;:\; c \in \mathrm{L}^\infty(\Omega, P)\,\}$, but we can not guarantee that there exists a function $c_k \in \mathrm{L}^\infty(\Omega, P)$ at which the infimum is attained, that is $J_k(c_k) = \alpha$. Only then we call α the minimum of $J_k(\cdot)$ over $\mathrm{L}^\infty(\Omega, P)$. Of course we can choose c^j such that it converges weak* to a function $c_* \in \mathrm{L}^\infty(\Omega, \widehat{P})$ but $J_k(c_*)$ may not be defined (since $c_*(x) \in \widehat{P}$ may not lie in P) or c_* may satisfy $J_k(c_*) > \alpha$ if $J_k(\cdot)$ is not weak* lower semi continuous.

It is exactly this phenomenon of nonattainement which leads to the formation of microstructure, that is the phase distributions c_k try to oscillate between different phases e_j such that on a macroscopic level one sees a phase mixture $c^* \in \mathrm{L}^\infty(\Omega, \widehat{P})$.

Neither in a real physical process nor in a mathematical approximation of (IP) we can expect that exact minimization of $I(t_k, \cdot) + \mathcal{D}(c_{k-1}, \cdot)$ occurs. Thus, we propose the following **approximate incremental problem** $(\mathrm{AIP})_\varepsilon$ where quasiminimal solutions are allowed.

(AIP)$_\varepsilon$ Given $c_0 \in \mathrm{L}^\infty(\Omega, P)$ find $c_1, \ldots, c_N \in \mathrm{L}^\infty(\Omega, P)$ such that

$$I(t_k, c_k) + \mathcal{D}(c_{k-1}, c_k) \le \varepsilon + \inf\{\, I(t_k, c) + \mathcal{D}(c_{k-1}, c) \;:\; c \in \mathrm{L}^\infty(\Omega, P)\,\}.$$

Clearly, this problem always has a solution and the question remains how the solutions behave for $\varepsilon \to 0$.

3 Simple one–dimensional examples

To illustrate the above ideas we consider the simplest nontrivial example which is given by a one–dimensional theory with $\Omega = (0, 1)$ which, for example, arises in plane shear or in uniaxial extension. However, our main purpose of investigating the one–dimensional case is to illustrate the effect of the extremum principle and the incremental formulations at the most simple but nontrivial case.

We assume that the material has two phases each with a quadratic energy $W_{e_i}(F) = (F - A_i)^2/H_i + B_i$. To simplify the analysis we let $A_1 = 0$, $A_2 = a$, $B_1 = 0$, $B_2 = b$, and $H_1 = H_2 = h$. (The problem considered here is a special case of the energy densities treated in Section 6.1.) There are no volume forces, and the boundary conditions are $u(t, 0) = 0$ (displacement given) and at $x = 1$ either $\Sigma(t, 1) = \lambda(t)$ (traction given) or $u(t, 1) = \ell(t)$ (displacement given). The elastic energy reads

$$\begin{aligned} E_{\mathrm{tract}}(t, c, u) &= \textstyle\int_0^1 W_{c(x)}(\partial_x u(t, x))\,\mathrm{d}x - \lambda(t) u(t, 1), \\ E_{\mathrm{displ}}(t, c, u) &= \textstyle\int_0^1 W_{c(x)}(\partial_x u(t, x))\,\mathrm{d}x. \end{aligned}$$

For given $c \in \mathrm{L}^\infty(\Omega, \{e_1, e_2\})$ we find the unique minimizer from $\partial_F W_{c(x)}(\partial_x u) = \lambda(t)$ and a simple calculation gives

$$I_{\mathrm{tract}}(t, c) = (1-\theta)(b - a\lambda(t)) - h\lambda(t)^2/4, \quad I_{\mathrm{displ}}(t, c) = (\ell(t) - a(1-\theta))^2/h + b(1-\theta).$$

The unique feature of this simple problem is that both I and $\mathcal{D}$ only depend on the ratio θ of the material occupying phase e_1, viz. $\int_0^1 c(x)\,\mathrm{d}x = \theta e_1 + (1-\theta)e_2$. It is not relevant at what points of the body Ω phase e_1 is located as long as the overall ratio θ is known.

For the dissipation we assume $\kappa_{1\to 2} = \kappa_{2\to 1} = \kappa$ then we have

$$\mathcal{D}(c_0, c) = \int_\Omega \frac{\kappa}{2} \|c_0(x) - c(x)\|_1 \,\mathrm{d}x \geq \kappa|\theta_0 - \theta|$$

where the lower bound is achieved if $c_0(x) \geq c(x)$ almost everywhere or $c(x) \geq c_0(x)$ almost everywhere. Since we incremental problem consists in minimizing $I + \mathcal{D}$ it is clear that we always want to use the lower bound, which can be achieved by taking $c(t, x) = e_1$ for $x \leq \theta(t)$ and e_2 else. However, even with fixed $\theta(t)$ there is a big nonuniqueness as we may have growing regions with phase e_2 of completely different shape.

3.1 The traction problem

We first treat the time continuous traction problem. We derive separately the condition arising from the energy inequality and the extremum principle. Writing $I_{\text{tract}}(t_2, \theta(t_2)) - I_{\text{tract}}(t_1, \theta(t_1))$ as the integral $\int_{t_1}^{t_2} [-(h\lambda/2 + a(1-\theta))\dot{\lambda} - (b - \lambda a)\dot{\theta}]\,\mathrm{d}t$ and comparing with the energy inequality gives

$$\int_{t_1}^{t_2} \left[\kappa|\dot{\theta}(t)| - (b - a\lambda(t))\dot{\theta}(t)\right] \mathrm{d}t \leq 0 \quad \text{for all } 0 \leq t_1 < t_2 \leq T.$$

Using the critical loads $\lambda^{\pm} = (b \pm \kappa)/a$, one sees that the energy inequality holds if and only if the following holds: if $\lambda(t) \neq \lambda^{\pm}$ then $\dot{\theta}(t) = 0$, if $\lambda(t) = \lambda^-$ then $\dot{\theta}(t) \geq 0$, and if $\lambda(t) = \lambda^+$ then $\dot{\theta} \leq 0$. Here we have to include the case that $\theta \in [0, 1]$ has jumps (and thus $\dot{\theta}$ is a delta distribution).

For the extremum principle we use $J(t, \theta, \vartheta) = -h\lambda^2/4 + (b - a\lambda)(1-\theta) + \kappa|\theta - \vartheta|$; and the condition $J(t, \theta(t), \vartheta) \geq J(t, \theta(t), \theta(t))$ for all $\vartheta \in [0, 1]$ is equivalent to

$$(b - a\lambda(t))(\theta(t) - \vartheta) + \kappa|\theta(t) - \vartheta| \quad \text{for all } \vartheta \in [0, 1].$$

This condition is satisfied if and only if

$$\begin{cases} \theta(t) = 1 & \text{if } \lambda < \lambda^-, \\ \theta(t) \in [0, 1] & \text{if } \lambda \in [\lambda^-, \lambda^+], \\ \theta(t) = 0 & \text{if } \lambda > \lambda^+. \end{cases}$$

We see that the extremum principle and the energy inequality determine the function $\theta(t)$ almost completely. For $\lambda \notin [\lambda^-, \lambda^+]$ the extremum principle determines θ. If $\lambda(t)$ changes inside of this interval then the energy inequality tells us that $\theta(t)$ remains constant. Only at the boundaries of the interval we have an indeterminacy, e.g. if $\lambda(t) = \lambda^+$ on $[t_1, t_2]$ then $\theta(t)$ can be chosen as any monotone decaying function (not necessarily continuous). In fact, we even have a nonuniqueness for the scalar function $\theta(t)$ if $\lambda(t)$ touches the boundaries of the interval from the inside, e.g. if $\lambda(t) = \lambda^+ - |t - t_2|$, then for any $1 \geq \theta_1 \geq \theta_2 \geq \theta_3 \geq 0$ the function θ with $\theta(t) = \theta_1$ for $t \leq t_1$, θ_2 for $t = t_2$, and θ_3 for $t > t_3$ is a solution.

Here we clearly see the hysteresis effect since for almost all times θ attains the value 0 or 1 and it switches between the two states at loads $\lambda^{\pm}$. This is like glass sliding on a rocking tray which is always at the border of the tray.

Having determined the set of solutions of (CP) we can now compare to the solutions of (IP). For $t=t_k$ we have to minimize

$$J_{\mathrm{tract}}(t,\theta_{k-1},\theta) = -k\lambda(t)^2/4 + (b{-}a\lambda(t))(1{-}\theta) + \kappa|\theta{-}\theta_{k-1}|$$

with respect to $\theta_k \in [0,1]$. We find the minimizers θ_k with

$$\begin{cases} \theta_k = 1 & \text{if } \lambda(t_k) < \lambda^-, \\ \theta_k \in [\theta_{k-1},1] & \text{if } \lambda(t_k) = \lambda^-, \\ \theta_k = \theta_{k-1} & \text{if } \lambda(t_k) \in [\lambda^-,\lambda^+], \\ \theta_k \in [0,\theta_{k-1}] & \text{if } \lambda(t_k) = \lambda^+, \\ \theta_k = 0 & \text{if } \lambda(t_k) > \lambda^+. \end{cases}$$

We see that (IP) produces exactly the solutions of the continuous problem. Both effects, of the energy inequality and of the extremum principle, are captured by (IP).

3.2 The displacement problem

The traction and the displacement problem are related by $\ell(t) = h\lambda(t)/2{+}(1{-}\theta(t))a$. Hence, in the traction problem the energy inequality reduces to

$$\int_{t_1}^{t_2} \Big[\kappa|\dot\theta(t)| - (b{-}2a(\ell(t){-}a[1{-}\theta(t)])/h)\dot\theta(t)\Big]\,\mathrm{d}t \le 0 \quad \text{for all } 0 \le t_1 < t_2 \le T.$$

This holds if and only if $\pm\dot\theta(t) \ge 0$ for $\ell(t){-}h(b \mp \kappa)/(2a) \le a(1{-}\theta(t))$. The stability principle is equivalent to

$$(b{-}2a\ell/h)(\theta{-}\vartheta) + a^2(\theta{-}\vartheta)(2{-}\theta{-}\vartheta) + \kappa|\theta{-}\vartheta| \ge 0 \quad \text{for all } \vartheta \in [0,1].$$

Using the piecewise quadratic form of this condition we find that the extremal condition is satisfied for $\theta(t) \in [0,1]$ if and only if

$$\min\{1, 1{+}(\ell^-{-}\ell(t))/a\} \le \theta(t) \le \max\{0, 1{+}(\ell^+{-}\ell(t))/a\}, \tag{3.1}$$

where $\ell^\pm = h(b \pm \kappa)/(2a)$.

The energy inequality together with the extremum principle determine the solution uniquely. If the bounds in (3.1) give several choices then the energy inequality forces the solution $\theta(t)$ to stay constant or to follow the bound which is attained (but only if it moves in the correct direction).

The incremental problem consists in minimizing

$$J_{\mathrm{displ}}(t_k,\theta_{k-1},\theta) = (\ell(t_k){-}a(1{-}\theta))^2/h + b(1{-}\theta) + \kappa|\theta{-}\theta_{k-1}|.$$

Because of the strict convexity of the functional in $\theta \in [0,1]$ the minimizer θ_k is unique. Using the function Θ_ρ defined in Appendix A we find $\theta_k = \Theta_{\kappa h/(2a^2)}(\theta_{k-1}, 1{+}hb/(2a^2){-}\ell(t_k)/a)$, which gives explicitly

$$\theta_k = \begin{cases} 0 & \text{if } \ell(t_k) \ge \ell^+{+}a, \\ 1{+}(\ell^+ - \ell(t_k))/a & \text{if } \ell(t_k) \in [\ell^+{+}a(1{-}\theta_{k-1}), \ell^+{+}a], \\ \theta_{k-1} & \text{if } \ell(t_k) \in [\ell^-{-}a(1{-}\theta_{k-1}), \ell^+{+}a(1{-}\theta_{k-1})], \\ 1{+}(\ell^- - \ell(t_k))/a & \text{if } \ell(t_k) \in [\ell^-, \ell^-{-}a(1{-}\theta_{k-1})], \\ 1 & \text{if } \ell(t_k) \le \ell^-. \end{cases}$$

From this explicit formula we see that the solution θ_k coincides with the solution $\widetilde{\theta}(t_k)$ of the following continuous-time problem. Define $\widetilde{\ell}(t)$ as any piecewise monotone interpolation of the points $(t_j, \ell(t_j))_{j=0,\dots,N}$. Then $\widetilde{\theta}(t)$ is the associated solution of (CP). Thus, we again found that (IP) and (CP) are properly connected in the sense that making the increments smaller in (IP) produces a sequence of solutions which converges to the solution of (CP).

4 Mathematical Approach

4.1 Weak limits and relaxation

We now return to the general problem and the approximate incremental problem $(\mathrm{AIP})_\varepsilon$ with solution $(c_1^\varepsilon, \dots, c_N^\varepsilon)$. In practice, one is often not interested in the details of c_k^ε for $\varepsilon \ll 1$ like the exact geometry of the microstructure of the phases. More relevant are global or averaged quantities like the energy $I(t_k, c_k^\varepsilon)$, the deformation $u_k^\varepsilon = \mathcal{U}(G(t_k), c_k^\varepsilon)$, or the macroscopic distribution of the volume fractions of the phases. Even when $c_k^\varepsilon(x)$ does not converge for $\varepsilon \to 0$, these quantities may converge when the the weak limit exists, $c_k^\varepsilon \overset{*}{\rightharpoonup} \widehat{c}_k$. This convergence is defined via

$$\lim_{\varepsilon\to 0} \int_{B_r(x_0)} c_k^\varepsilon(x)\,\mathrm{d}x = \int_{B_r(x_0)} \widehat{c}_k(x)\,\mathrm{d}x \quad \text{for all } B_r(x_0) \subset \Omega.$$

The weak limit $\widehat{c}_k$ takes its values no longer in $P = \{e_1, \dots, e_n\}$ but in its convex hull $\widehat{P}$, that is $\widehat{c}_k \in \mathrm{L}^\infty(\Omega, \widehat{P})$. Thus, the functional

$$J_k(a, c) = I(t_k, c) + \mathcal{D}(a, c), \quad a, c \in \mathrm{L}^\infty(\Omega, P),$$

has to be extended to a functional $\widehat{J}_k : \mathrm{L}^\infty(\Omega, P) \times \mathrm{L}^\infty(\Omega, \widehat{P}) \to I\!R$ such that

$$\widehat{J}_k(a, \widehat{c}) = \inf\{ \liminf_{\varepsilon\to 0} J(a, c^\varepsilon) \;:\; \text{ all sequences } c^\varepsilon \in \mathrm{L}^\infty(\Omega, P) \text{ with } c^\varepsilon \overset{*}{\rightharpoonup} \widehat{c} \text{ for } \varepsilon \to 0 \;\}.$$

Such a functional is called the relaxation of $J_k(a, \cdot)$, see [Dac89, Rou97]. While the relaxation of $J_k(a, c)$ in c is clear, it is open how the extension from $a \in \mathrm{L}^\infty(\Omega, P)$ to $\widehat{a} \in \mathrm{L}^\infty(\Omega, \widehat{P})$ has to be done in order to have a proper connection between the following **relaxed incremental problem** (RIP) and the original incremental problem.

(RIP) Given $c_0 \in \mathrm{L}^\infty(\Omega, P)$ find $\widehat{c}_1, \dots, \widehat{c}_N \in \mathrm{L}^\infty(\Omega, \widehat{P})$ such that

$$\widehat{J}_k(\widehat{c}_{k-1}, \widehat{c}_k) = \inf\{ \widehat{J}_k(\widehat{c}_{k-1}, \widehat{c}) \;:\; \widehat{c} \in \mathrm{L}^\infty(\Omega, \widehat{P}) \}.$$

It remains to manifest the relations between (RIP) and (IP) (or $(\mathrm{AIP})_\varepsilon$ resp.). Of course, (RIP) is only meaningful if at least one of the following two questions (or appropriate variants of them) can be answered affirmative.

Question 1: Let $(c_1^\varepsilon, \dots, c_N^\varepsilon)$ solve $(\mathrm{AIP})_\varepsilon$ such that $c_k^\varepsilon \overset{*}{\rightharpoonup} \widehat{c}_k$ for $\varepsilon \to 0$. Does $(\widehat{c}_1, \dots, \widehat{c}_N)$ solve (RIP)?

Question 2: Let $(\widehat{c}_1, \dots, \widehat{c}_N)$ solve (RIP). Does there exist solutions $(c_1^\varepsilon, \dots, c_N^\varepsilon)$ of $(\mathrm{AIP})_\varepsilon$ such that $c_k^\varepsilon \overset{*}{\rightharpoonup} \widehat{c}_k$ for $\varepsilon \to 0$?

4.2 Separate relaxation

The abstract relaxation procedure described in the previous section used the functional $J_k(a,c) = I(t_k,c)+\mathcal{D}(a,c)$. At the present the proper relaxation of this sum is not known except for special cases, like the one–dimensional case treated below. Hence we make a modelling assumption at this point which amounts in mathematical terms in the fact that we relax $J(\cdot,\cdot)$ in both arguments, that is $\widehat{J} : \mathrm{L}^\infty(\Omega,\widehat{P})^2 \to I\!R$ is defined via

$$\widehat{J}_k(\widehat{a},\widehat{c}) = \inf\{\, \liminf_{\varepsilon\to 0} J(a^\varepsilon,c^\varepsilon) \;:\; \text{all sequences } a^\varepsilon, c^\varepsilon \in \mathrm{L}^\infty(\Omega,P) \text{ with } a^\varepsilon \overset{*}{\rightharpoonup} \widehat{a},\; c^\varepsilon \overset{*}{\rightharpoonup} \widehat{c} \text{ for } \varepsilon\to 0 \,\}.$$

In fact, it is shown in [The98] that this simultaneous relaxation is the same as the sum of the separate relaxations of $I(t_k,\cdot)$ and $\mathcal{D}(\cdot,\cdot)$. This is not surprising, since the two functionals have a different dependence on c. The dissipation $\mathcal{D}(a,c)$ depends on a and c only through the volume of the sets $\{\, x\in\Omega \,:\, (a(x),c(x)) = (e_j,e_k)\,\}$ but not on the particular microstructure. The energy $I(t_k,c)$ is very sensitive to the microstructure of c even when the volume fractions of the phases are kept fixed; a fact which will be seen more explicitly below when the mixing function is defined.

Mechanically, the assumption that the relaxation can be done separately can be interpreted in a way that the geometry of the microstructure should not change too much from one timestep to the next. In fact, the only two cases where the Question 2 above can be answered positively are cases where the geometry microstructure can be fixed, namely in the one-dimensional case ([Mie98])) and in the case of two linearly elastic phases ([The98]).

First we recall the definition of quasiconvexity which plays a central role in the existence theory for minimizers in the calculus of variations. A function W is called quasiconvex at F if and only if

$$\fint_\Omega W(F+\nabla\phi(y))\,\mathrm{d}y \geq W(F) \quad \text{for all } \phi\in \mathrm{W}^{1,p}_0(\Omega).$$

Throughout we use the notation $\fint_A f(x)\,\mathrm{d}x = \frac{1}{\mathrm{vol}(A)}\int_A f(x)\,\mathrm{d}x$.

Further on we always assume that the energy densities W_{e_j} of the pure phases are quasiconvex in this sense. Considering a small ball of material $B_r(x_0) = \{\, x\in\Omega \,:\, |x-x_0| < r\,\}$ where the phase distribution is given by $\widehat{c} = \fint_{B_r(x_0)} c(x)\,\mathrm{d}x$. We now allow for a suitable rearrangement of the phases without changing the average and we also allow a perturbation ϕ of the deformation which vanishes on the boundary of the ball. For small r the perturbation can be understood as a microscopic adjustment which does not affect the macroscopic deformation. We are lead to the **mixture function**

$$\widehat{W}_{\widehat{c}}(F) \overset{\text{def}}{=} \inf\Big\{ \fint_B W_{c(y)}(F+\nabla\phi(y))\,\mathrm{d}y \;:\; \phi\in \mathrm{W}^{1,p}_0(B),\; c\in \mathrm{L}^\infty(B,P),\; \fint_B c(y)\,\mathrm{d}y = \widehat{c} \Big\} \tag{4.2}$$

which was already defined in [Koh91] as a tool to study the quasiconvexifications of $\min\{\, W_{e_j}(F) \,:\, j=1,\dots,n\,\}$. In this work, $\widehat{W}_{\widehat{c}}(F)$ itself plays a central role and is called the quasiconvexification with fixed phase fractions.

Note that the set $B = B_r(x_0)$ can in fact be replaced by any open set. We now have defined a function $\widehat{W}_{\widehat{c}}(F)$ for $(\widehat{c},F) \in \widehat{P}\times I\!R^{d\times d}$ which satisfies $\widehat{W}_{e_j}(F) = W_{e_j}(F)$ since

W_{e_j} was assumed to be quasiconvex. Thus, $\widehat{W}$ contains information on the mixture theory without the addition of new physics. In general the minimum $\widehat{W}_{\widehat{c}}(F)$ is not achieved, but one needs a minimizing sequence c^ε which tells us that certain microstructures are needed to minimize the energy under given phase fractions.

In Proposition 4.2 we state that $\widehat{P} \ni \widehat{c} \mapsto \widehat{W}_{\widehat{c}}(F)$ is convex for fixed F and that $\mathbb{R}^{d\times d} \ni F \mapsto \widehat{W}_{\widehat{c}}(F)$ is quasiconvex for fixed $\widehat{c}$. However, even for W_{e_j} which are convex in F we cannot expect that $\widehat{W}_{\widehat{c}}(F)$ is convex in $(\widehat{c}, F)$ as is seen be the simplest relevant example, namely the quadratic one–dimensional case with two phases: $\widehat{W}_{\theta e_1+(1-\theta)e_2}(F) = \frac{1}{h}(F-a\theta)^2 + b\theta$.

Similarly we can define a relaxation of the function $D(a,c)$ which is defined on $P\times P$ only . For $(\widehat{a},\widehat{c}) \in \widehat{P}\times\widehat{P}$ we set

$$\widehat{D}(\widehat{a},\widehat{c}) = \inf\{ \sum_{j,i=1}^{n} m_{ji}\kappa_{j\to i} \;:\; m_{ji}\geq 0,\; \sum_{i=1}^{n} m_{ji} = \widehat{a}\cdot e_j,\; \sum_{j=1}^{n} m_{ji} = \widehat{c}\cdot e_i \}. \tag{4.3}$$

Clearly $\widehat{D}$ is obtained by minimizing $\mathcal{D}(a,c)$ over $a,c\in \mathrm{L}(B,P)$ under the constraints $\widehat{a} = ⨍_B a(y)\,\mathrm{d}y$ and $\widehat{c} = ⨍_B c(y)\,\mathrm{d}y$. The coefficients m_{ji} in (4.3) are simply the relative measures of the sets $\{\, y\in B \,:\, a(y)=e_j,\; c(y)=e_i \,\}$. Using $\kappa_{j\to j}=0$, $\kappa_{\min} = \min\{\, \kappa_{j\to i} \,:\, j\neq i\,\}$, and $\kappa_{\max} = \max\{\, \kappa_{j\to i} \,:\, j\neq i\,\}$, we immediately find

$$\frac{\kappa_{\min}}{2}\|\widehat{a}-\widehat{c}\|_1 \leq \widehat{\mathcal{D}}(\widehat{a},\widehat{c}) \leq \frac{\kappa_{\max}}{2}\|\widehat{a}-\widehat{c}\|_1 \quad \text{where } \|\widehat{b}\|_1 \stackrel{\text{def}}{=} \int_\Omega \sum_{j=1}^{n} |\widehat{b}\cdot e_j|\,\mathrm{d}x.$$

We also have

$$\widehat{D}(e_j,\widehat{c}) = \sum_{i=1}^{n} (\widehat{c}\cdot e_i)\kappa_{j\to i}. \tag{4.4}$$

Proposition 4.1
The function $\widehat{D} : \widehat{P}\times\widehat{P} \to [0,\infty)$ is convex, that is

$$\widehat{D}(\theta\widehat{a}_1+(1-\theta)\widehat{a}_2, \theta\widehat{c}_1+(1-\theta)\widehat{c}_2) \leq \theta\widehat{D}(\widehat{a}_1,\widehat{c}_1) + (1-\theta)\widehat{D}(\widehat{a}_2,\widehat{c}_2).$$

If D satisfies the triangle inequality (2.9), then so does $\widehat{D}$ and there exists a function $\Delta : \mathbb{R}^n \to [0,\infty)$ which is homogeneous of degree 1 (that is $\Delta(\alpha\widehat{b}) = \alpha\Delta(\widehat{b})$ for all $\alpha\geq 0$ and $\widehat{b}\in\mathbb{R}^n$) such that $\widehat{D}$ has the form

$$\widehat{D}(\widehat{a},\widehat{c}) = \Delta(\widehat{c}-\widehat{a}) \quad \textit{for all } \widehat{a},\widehat{c}\in\widehat{P}. \tag{4.5}$$

Proof: Consider $\widehat{a}_i, \widehat{c}_i \in \widehat{P}$ and let $m_{jk}^{(i)}$ be the minimizers in the definition of $\widehat{\mathcal{D}}(\widehat{a},\widehat{c}_i)$ for $i=1,2$, that is $m_{jk}^{(i)}\geq 0$, $\sum_{l=1}^{n} m_{jl}^{(i)} = \widehat{a}_i\cdot e_j$, and $\sum_{j=1}^{m} m_{jl}^{(i)} = \widehat{c}_i\cdot e_l$. Then, $m_{jl}^{(3)} = \theta m_{jl}^{(1)} + (1-\theta)m_{jl}^{(2)}$ forms an admissible set in the definition of $\widehat{\mathcal{D}}(\theta\widehat{a}_1+(1-\theta)\widehat{a}_2, \theta\widehat{c}_1+(1-\theta)\widehat{c}_2)$, which gives the desired result after separating the minimum into the weighted sum of two minima.

The triangle inequality follows by a straight forward use of the definition of $\widehat{D}$.

The proof of the representation (4.5) involves the standard duality theory for the linear transport problem as developed in the textbooks [Gal60, Gas58]. This theory implies immediately the representation

$$\widehat{D}(\widehat{a},\widehat{c}) = \max\{\, \mu\cdot\widehat{c} - \nu\cdot\widehat{a} \;:\; \mu,\nu\in\mathbb{R}^n,\; \mu\cdot e_j - \nu\cdot e_i \leq \kappa_{i\to j} \text{ for all } i,j \,\}.$$

Our aim is to show that in our special situation it is sufficient to take $\nu=\mu$ which gives the function

$$\Delta(\widehat{c}-\widehat{a})=\max\{\,\mu\cdot(\widehat{c}-\widehat{a})\ :\ \mu\in I\!R^n,\ \mu\cdot e_j-\mu\cdot e_i\le\kappa_{i\to j}\text{ for all }i,j\,\}.$$

To this end we employ the following standard optimality condition. If (m_{ij}) is a minimizer in (4.3) and (μ,ν) a maximizer in the dual formulation then

$$m_{ij}>0\text{ implies }\kappa_{i\to j}=\mu\cdot e_j-\nu\cdot e_i.$$

Thus, using $\kappa_{j\to j}=0$ we are finished if we can show that $m_{jj}=0$ for all $j=1,\dots,n$.

For this purpose we use the triangle inequality. It guarantees that it is always possible to find a minimizer (m_{ij}) in (4.3) which satisfies

$$m_{ii}=\sigma_i\overset{\text{def}}{=}\min\{\widehat{a}\cdot e_i,\widehat{c}\cdot e_i\}\text{ for }i=1,\dots,n. \tag{4.6}$$

In fact, if this would not be the case for some i_0 then there exist j_0 and k_0 such that $\delta=\min\{m_{i_0j_0},m_{k_0i_0}\}\in(0,\sigma_{i_0}-m_{i_0i_0}]$. By the triangle inequality it is advantageous, for minimizing $\sum\kappa_{i\to j}m_{ij}$, to increase $m_{i_0i_0}$ and $m_{k_0j_0}$ by $\delta>0$ and decrease $m_{i_0j_0}$ and $m_{k_0i_0}$ by the same amount. Clearly after a finite number of such operations we achieve $\sigma_{i_0}=m_{i_0i_0}$.

Using identity (4.6) together with the extremality condition we conclude $\mu=\nu$ in the dual problem whenever $\widehat{a}$ and $\widehat{c}$ have positive coordinates. Then, the desired relation $\widehat{D}(\widehat{a},\widehat{c})=\Delta(\widehat{c}-\widehat{a})$ follows. By continuity of $\widehat{D}$ and Δ it immediately extends to all of $\widehat{P}\times\widehat{P}$. QED

Using these two relaxed functionals we can now postulate a relaxed formulation of the problem (IP). For $\widehat{a},\widehat{c}\in\mathrm{L}^\infty(\Omega,\widehat{P})$ we define

$$\widehat{I}(t,\widehat{c})=\inf\{\int_\Omega\widehat{W}_{\widehat{c}(x)}(\nabla u(x))\,\mathrm{d}x-\langle G(t),u\rangle\ :\ u\in V\,\},\quad \widehat{\mathcal{D}}(\widehat{a},\widehat{c})=\int_\Omega\widehat{D}(\widehat{a}(x),\widehat{c}(x))\,\mathrm{d}x$$

and postulate the following relaxed incremental problem

> **(RIP)** Given $c_0\in\mathrm{L}^\infty(\Omega,P)$ find $\widehat{c}_1,\dots,\widehat{c}_N\in\mathrm{L}^\infty(\Omega,\widehat{P})$ such that
>
> $$\widehat{I}(t_k,\widehat{c}_k)+\widehat{\mathcal{D}}(\widehat{c}_{k-1},\widehat{c}_k)=\inf\{\,\widehat{I}(t_k,\widehat{c})+\widehat{\mathcal{D}}(\widehat{c}_{k-1},\widehat{c})\ :\ \widehat{c}\in\mathrm{L}^\infty(\Omega,\widehat{P})\,\}.$$

To see that the relaxed problem has a solution we state some important properties of the mixture function, see [Mie98] for the proof.

Proposition 4.2
(a) The mixture function $\widehat{W}_{\widehat{c}}(F)$ as defined in (4.2) is convex in $c\in\widehat{P}$ for F fixed, and it is quasiconvex in F for $\widehat{c}$ fixed.
(b) For continuous $m:\widehat{P}\to I\!R$ define $\Psi(F)=\min\{\,\widehat{W}_{\widehat{c}}(F)+m(\widehat{c})\ :\ \widehat{c}\in\widehat{P}\,\}$. Then, for convex $m:\widehat{P}\to I\!R$ the function $F\mapsto\Psi(F)$ is quasiconvex.

It has to be noted that quasiconvexity is an important property in the theory of the calculus of variations. It is necessary for general existence results for minimizers and it is also sufficient when the integrand satisfies further technical assumptions, see [Dac89, AcF84]. The property stated in (b) will be especially useful to establish existence of solutions for (RIP) when m is taken as $\widehat{D}(\widehat{a}(x),\cdot)$.

For general existence results for (RIP) we refer to [Mie98]; there it is also shown that the one–dimensional case is exceptional since (RIP) as well as (IP) always have solutions. In Section 6.4 we give an example showing that in general (RIP) has a solution when (IP) has none. Sofar, a rigorous connection between (IP) and (RIP) via (AIP) is only know in the (trivial) one–dimensional case, see [Mie98] and in the case of linearized elasticity with two phases with the same elastic moduli. The following result is established in [The98]; it gives a positive answer to the Question 2 from above.

Theorem 4.3
Let $d \geq 1$, $n=2$ and $\mathbf{C}$ be a positive elasticity tensor, i.e.,

$$\langle \mathbf{C}E, E\rangle = \sum_{i,j,k,l=1}^{d} \mathbf{C}_{ijkl}E_{ij}E_{kl} \geq \alpha \|E\|^2 \quad \text{for } E \in S(d)$$

with $\alpha > 0$, where $E = \frac{1}{2}(F + F^T) - I$ and $E, A_i \in S(d) = \{\, M \in I\!R^{d\times d} \,:\, M = M^T \,\}$, the set of symmetric matrices. Denote by $\langle E, A\rangle$ the scalar product $\sum_{i,j} E_{ij}A_{ji}$. If the stored energy density functions W_{e_1} and W_{e_2} satisfy

$$W_{e_i}(F) = \frac{1}{2}\langle \mathbf{C}(E - A_i), E - A_i\rangle + B_i, \tag{4.7}$$

then for every time discretization there exists a solution $(c_{k,\varepsilon})_{k=1\dots N}$ to the approximate incremental problem (AIP) which converges to a solution $(\widehat{c}_k)_{k=1\dots N}$ of the relaxed incremental problem (RIP) as $\varepsilon \to 0$.

A major advantage of (RIP) is that it can be solved efficiently as $(\widehat{c}_k, u_k)$ have to solve a variational problem of 'inf inf' type, where the functional is an integral containing $\widehat{c}$ only pointwise. Define $\widehat{E}(t,\widehat{c},u) = \int_\Omega \widehat{W}_{\widehat{c}(x)}(\nabla u)\,\mathrm{d}x - \langle G(t_k), u\rangle$, then $(\widehat{c}_k, u_k)$ have to satisfy

$$\widehat{E}(t,\widehat{c}_k,u_k) + \widehat{\mathcal{D}}(\widehat{c}_{k-1},\widehat{c}_k) = \inf\{\, \widehat{E}(t,\widehat{a},v) + \widehat{\mathcal{D}}(\widehat{c}_{k-1},a) \,:\, \widehat{a} \in \mathrm{L}^\infty(\Omega,\widehat{P}),\ v \in V \,\}.$$

Since $\widehat{E}(t,\widehat{a},v) + \widehat{\mathcal{D}}(\widehat{c}_{k-1},a)$ can be written as one integral over Ω with the integrand $\widehat{W}_{\widehat{c}(x)}(\nabla u(x)) + \widehat{D}(\widehat{a}(x),\widehat{c}(x))$ it is advantageous to minimize first with respect to $\widehat{c}$ which can be done pointwise in $x \in \Omega$.

For this purpose define

$$\widehat{\Psi}(\widehat{a},F) = \min\{\, \widehat{W}_{\widehat{c}}(F) + \widehat{D}(\widehat{a},\widehat{c}) \,:\, \widehat{c} \in \widehat{P} \,\}, \tag{4.8}$$

where, by continuity of $\widehat{W}_{(\cdot)}(F) + \widehat{D}(\widehat{a},\cdot)$, the minimum is achieved at $\widehat{c} = \widehat{C}(\widehat{a},F)$, that is $\widehat{\Psi}(\widehat{a},F) = \widehat{W}_{\widehat{C}(\widehat{a},F)}(F) + \widehat{D}(\widehat{a},\widehat{C}(\widehat{a},F))$. Let

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

then (RIP) can be formulated as follows

(RIP)' Given $c_0 \in \mathrm{L}^\infty(\Omega, P)$ find $(\widehat{c}_1, u_1), \ldots, (\widehat{c}_N, u_N) \in \mathrm{L}^\infty(\Omega, \widehat{P}) \times V$ such that

$$\widehat{\mathcal{E}}(t_k, \widehat{c}_{k-1}, u_k) = \inf\{\, \widehat{\mathcal{E}}(t_k, \widehat{c}_{k-1}, v) \;:\; v \in V \,\} \text{ and } \widehat{c}_k(x) = \widehat{C}(\widehat{c}_{k-1}(x), \nabla u_k(x)).$$

The formulation of (RIP)' has the major advantage that it reduces to a simple variational problem for the variable $u_k \in V$. It can be shown that $F \mapsto \widehat{\Psi}(\widehat{a}, F)$ is quasiconvex, hence the existence of a minimizer is clear. The important message is that the function $\widehat{\Psi}(\widehat{a}, F)$ is in principle completely determined from the pure energy densities $W_{e_j}(F)$ and the dissipation coefficients $\kappa_{i\to j} = D(e_i, e_j)$. It can be calculated either analytically or numerically before even starting to solve the incremental problem (RIP). We give explicit calculations in Section 6.3.

4.3 The relaxed time-continuous problem

Comparing the (unrelaxed) time-continuous and incremental problem it is natural to go back from the relaxed incremental problem to a relaxed time-continuous problem. Its formulation uses the relaxed energy inequality

$$\widehat{I}(t_2, \widehat{c}(t_2)) + \widehat{\mathrm{Diss}}(\widehat{c}; t_1, t_2) \le \widehat{I}(t_1, \widehat{c}(t_1)) - \int_{t_1}^{t_2} \langle \dot{G}(t), u(t) \rangle \,\mathrm{d}t, \tag{4.9}$$

where $u(t)$ is the minimizer of $\widehat{E}(t, \widehat{c}(t), \cdot)$ or $\widehat{\mathcal{E}}(t, \widehat{c}(t), \cdot)$. The relaxed dissipation integral is calculated as in (2.4) but with $\mathcal{D}$ replaced by $\widehat{\mathcal{D}}$.

Let us summarize this section's results. We have replaced the time-continuous formulation by a time-discrete approximation scheme. In order to achieve existence of solutions at each time step it became necessary to relax the minimization problems to generalized (microstructure) solutions. At least fomally, we can now interprete the incremental solutions of (RIP) as approximations of the solutions of a time-contontinuous problem (RCP). In fact it has exactly the same form as (CP) except that we have introduced the relaxation sign $\widehat{\cdot}$ on all the variables and functions.

(RCP) Given $\widehat{c}_0 \in \mathrm{L}^\infty(\Omega, \widehat{P})$ find $\widehat{c} : [0, T] \to \mathrm{L}^\infty(\Omega, \widehat{P})$ with $\widehat{c}(0) = \widehat{c}_0$ such that the relaxed energy inequality (4.9) and the stability condition

$$\widehat{I}(t, \widehat{a}) + \widehat{\mathcal{D}}(\widehat{c}(t), \widehat{a}) \ge \widehat{I}(t, \widehat{c}(t)) \quad \text{for all } \widehat{a} \in \mathrm{L}^\infty(\Omega, \widehat{P})$$

holds.

For the general case it is an open problem to show that the incremental solutions of (RIP) converge to solutions of (RCP) if the time increments converge to 0. However, we have the following partial result. The key feature which helps to extract a a converging subsequence is that the dissipation bounds the variation of the state function $\widehat{c}$.

Theorem 4.4
Consider a continuously differentiable loading function $G : [0, T] \to V^*$, a sequence of time discretizations $0 = t_0^n < t_1^n \ldots t_{N(n)}^n = T$ whose fineness $\max_{k=1\ldots N(n)} |t_k^n - t_{k-1}^n|$ tends to 0 as $n \to \infty$, and assume $\kappa_{i\to j} > 0$ for $i \ne j$. Let $(c_k^n)_{k=0,\ldots,N(n)}$ be the solution of (RIP) and consider the piecewise constant function $\widehat{c}^n = \sum_{i=1}^{N(n)} \widehat{c}_k^n \cdot \chi_{[t_{k-1}^n, t_k^n)}$. Then there exists a subsequence (n_j) and a process $\widehat{c}^\infty : [0, T] \to \widehat{P}$ such that

1. *$\int_0^T \|\widehat{c}^{n_j}(t) - \widehat{c}^\infty(t)\|_{W^{-1,1}(\Omega)}\,\mathrm{d}t \to 0$ for $j \to \infty$, where $W^{-1,1}(\Omega)$ denotes the dual space of $W_0^{1,\infty}(\Omega)$, the set of Lipschitz–continuous functions which vanish at the boundary.*

2. *We have $\widehat{c}^\infty(0) = c_0$ and for almost every $t \in [0,T]$ we have $\widehat{c}^{n_j}(t) \stackrel{*}{\rightharpoonup} \widehat{c}^\infty(t)$.*

3. *$\widehat{\mathrm{Diss}}(\widehat{c}^\infty; t_1, t_2) \le \limsup_{j\to\infty} \widehat{\mathrm{Diss}}(\widehat{c}^{n_j}; t_1, t_2)$ for all t_1, t_2 with $0 \le t_1 \le t_2 \le T$.*

4. *$\widehat{c}^\infty$ satisfies the weak energy inequality.*

The existence of admissible processes in the case $d > 1$ is open.

Proof: To avoid difficulties in the functional analytic setting we shall assume that for an arbitrary $v \in V$ the space $V - v$ is a reflexive Banach space. For a solution $\widehat{c}^n_k$, u^n_k of the relaxed incremental problems (RIP)

$$(\widehat{c}^n_k, u^n_k) = \mathrm{argmin}_{\widehat{c},u} \int_\Omega \widehat{W}_{\widehat{c}(x)}(\nabla u(x))\,\mathrm{d}x - \langle G(t^n_k), u\rangle + \widehat{\mathcal{D}}(\widehat{c}^n_{k-1}, \widehat{c}),$$

we define $G^n \in C_{\mathrm{lip}}([0,T], V^*)$, $\widehat{c}^n \in BV([0,T], L^1(\Omega))$ and $u^n_k \in L^\infty([0,T], V)$, where C_{lip} is the space of Lipschitz continuous functions.

$$\begin{array}{rcl} G^n(t) &=& G(t^n_k) + \frac{t-t^n_k}{t_{k+1}-t_k}(G(t^n_{k+1}) - G(t^n_k)) \text{ for } x \in [t^n_{k+1} - t^n_k], \\ \widehat{c}^n &=& \sum_{i=0}^{N(n)} \widehat{c}^n_k \cdot \chi_{[t^n_{k+1}, t^n_k)}, \\ u^n &=& \sum_{i=0}^{N(n)} u^n_k \cdot \chi_{[t^n_{k+1}, t^n_k)}. \end{array}$$

G^n arises from a piecewise linear interpolation process, c^n and u^n are piecewise constant. Elementary calculations show that $\|G^n\|_{BV} \le \|G\|_{BV}$. See Appendix B for the definition of $BV([0,T], X)$ and $\|\cdot\|_{BV}$.

For Lipschitz continuous loadings G the total energy of the system at time t is

$$\Phi(c, G, u, t) = \int_\Omega \widehat{W}_{\widehat{c}(t)}(\nabla u(t))\,\mathrm{d}x - \langle G(t), u(t)\rangle + \int_0^t \langle \dot{G}(s), u(s)\rangle\,\mathrm{d}s + \widehat{\mathrm{Diss}}(\widehat{c}; 0, t)$$

where $\widehat{\mathrm{Diss}}(\widehat{c}; 0, t)$ is the supremum of $\sum_i \widehat{\mathcal{D}}(\widehat{c}(s_{i-1}), \widehat{c}(s_i))$ over the partitions $\{s_i\}$ of the time interval $[0,T]$. Since every $\widehat{c}^n_k$ is the solution to a minimization problem one can derive the strong energy inequality for the solutions to the relaxed incremental problems:

$$\Phi(\widehat{c}^n, G^n, u^n, t) \le \Phi(\widehat{c}^n, G^n, u^n, s) \text{ if } t \ge s,$$

thus $t \mapsto \Phi(\widehat{c}^n, G^n, u^n, t)$ is a decreasing function. The strong energy inequality immediately gives an estimate for the total dissipation

$$\widehat{\mathrm{Diss}}(\widehat{c}^n; 0, T) \le \hat{I}(0, \widehat{c}_0) + \langle G(T), u(T)\rangle - \int_0^T \langle \dot{G}^n(s), u^n(s)\rangle\,\mathrm{d}s,$$

where we have assumed that the stored energy functions $W_{e_i}(\cdot)$ are nonnegative. From the existence theory for the elastic deformation u one obtains an a–priori estimate $\|u\|_V \le C\left(\sup_{t\in[0,T]} \|G(t)\|\right)$ where C depends only on the stored energy functions, the boundary conditions specified by V, the space of admissible deformations, and the external loading given by G. For a precise specification of C see [Mie98]. Thus

$$\widehat{\mathrm{Diss}}(\widehat{c}^n; 0, T) \le \hat{I}(0, \widehat{c}_0) + C(2 + \tfrac{1}{T})\|G\|_{BV},$$

where $\sup_{t\in[0,T]} \|G(t)\| \leq (1+\frac{1}{T})\|G\|_{BV}$ has been used. Recalling that $\widehat{\mathcal{D}}(\widehat{a},\widehat{b}) \geq \frac{\kappa_{\min}}{2}\|\widehat{a}-\widehat{b}\|_{L^1(\Omega)}$ Theorem B.4 implies the existence of $\widehat{c}^\infty \in BV([0,T],L^1(\Omega))$ and a subsequence (not relabeled) so that $\lim_{n\to\infty}\int_0^T \|\widehat{c}^n(t)-\widehat{c}^\infty(t)\|_{W^{-1,1}(\Omega)}\,\mathrm{d}t = 0$ holds.

Extracting a further subsequence if necessary, and applying the usual compactness results in L^p–spaces one finds that also u^n converges weakly in $L^2([0,T],V_w)$ to a function u^∞. From the sequence of nonincreasing functions $t \mapsto \Phi(c^n,G^n,u^n,t)$ a further subsequence which converges pointwise to a nonincreasing function $t\mapsto K(t)$ can be extracted. Without loss of generality we assume that the loading program $G|_{t\in[0,\varepsilon]}$ is constant for a small number $\varepsilon > 0$. From this assumption follows that $t=0$ is a Lebesgue point of c. Using the weak* lower semicontinuity of I and $\mathcal{D}$ one can easily show that for almost every $t>0$ the weak energy inequality

$$\Phi(\widehat{c},G,u,t) \leq K(t) \leq K(0) = \Phi(\widehat{c},G,u,0)$$

holds, thus $\Phi(\widehat{c},G,u,t)$ satisfies the weak energy inequality. QED

The previous theorem can only be considered as a preliminary result as it has two shortcomings. First we cannot derive the strong energy inequality, second we cannot conclude the stablity of the limit process. The latter problem arises from the fact that it is not clear whether the set $\mathcal{S}(t)$ of stable states as time t is weakly closed:

$$\mathcal{S}(t) = \{\, \widehat{c} \in \mathrm{L}^\infty(\Omega,\widehat{P}) \;:\; \widehat{I}(t,a) + \widehat{\mathcal{D}}(\widehat{c},\widehat{a}) \geq \widehat{I}(t,\widehat{c}) \text{ for all } \widehat{a}\in \mathrm{L}^\infty(\Omega,\widehat{P})\,\}.$$

Clearly $\widehat{I}(t,\cdot)$ and $\widehat{\mathcal{D}}$ are continuous in the strong toplogy (even in the norm topology of $\mathrm{L}^2(\Omega,I\!R^n)$), hence the set $\mathcal{S}(t)$ is strongly closed. However, this is not sufficient. In the one–dimensional case it is shown in [Mie98] that $\widehat{I}(t,\cdot)$ is even weak* continuous which obviously implies weak* closedness of $\mathcal{S}(t)$. For the general case we only have the following conjecture

Conjecture. Under the assumptions of Theorem 4.3 the set $\mathcal{S}(t)$ is weak* closed.

If this conjecture turns out to be true then we are able to conclude that the limit $\widehat{c}^\infty$ is also stable. Thus, we almost solved the relaxed time-continuous problem for this special case; only the strong energy inequality is missing.

5 Pointwise stability results

5.1 Stability against nucleation of new phases

Conditions on the phase function can only be obtained from the minimizing properties of the function c postulated in (IP) or $\widehat{c}$ in (RIP). We now derive necessary conditions for c satisfying the minimizing principles by constructing suitable comparison processes. This will only be done at a point $x_0\in\Omega$ where $c(x)=e_i$ in a neighborhood of x_0, that is we need a pure phase. We introduce locally a nucleus of material which may consist of different phases and check whether this nucleus is favorable compared to the original phase e_i.

A candidate for a nucleus of new phases at x_0 is given by $c_{\mathrm{nucl}} \in \mathrm{L}^\infty(B_1(0),P)$ and some for some small radius $r>0$. The average phase distribution of the nucleus is given by $\widehat{c} = \fint_{B_1(0)} c(x)\,\mathrm{d}x \in \widehat{P}$. The comparison phase function $\widetilde{c}(t)$ is given by

$$\widetilde{c}(x) = \begin{cases} c_{\mathrm{nucl}}((x-x_0)/r) & \text{for } |x-x_0| < r, \\ e_i & \text{else.} \end{cases}$$

Such a change in the phase function generates dissipation and we have to check whether an associated gain in the energy is accompanied. Since we only want to derive local properties not involving the global behavior of the boundary value problem, we try to accommodate the changes by an according change in u which is restricted to the ball $B_r(x_0)$, namely $\widetilde{u}(x) = u(x) + r\phi((x-x_0)/r)$ with $\phi \in \mathrm{W}_0^{1,p}(B_1(0))$. Using $\nabla\widetilde{u} = \nabla u + (\nabla\phi)((x-x_0)/r)$ and the fact that the contribution of this correction to the energy of the external loading decays faster than r^d we obtain the following result.

Definition 5.1
We define the function

$$X(F, e_i, \widehat{c}) = \widehat{W}_{\widehat{c}}(F) + \widehat{D}(e_i, \widehat{c}) - W_{e_i}(F).$$

We say that (F, e_i) is a **stable pure state** *for the family $(W_{e_j})_{j=1,\ldots,n}$ if $X(F, e_i, \widehat{c}) \geq 0$ for all $\widehat{c} \in \widehat{P}$.*

The function X can be evaluated explicitly if $\widehat{c} = e_j$ by using the extremal property that $\fint_\Omega \widehat{c}(x)\,\mathrm{d}x = e_j$ automatically $\widehat{c}(x) = e_j$ almost everywhere implies. The following properties of X are immediate.

Lemma 5.2
(a) The function $X(F, e_i, \cdot) : \widehat{P} \to I\!R$ is convex.

(b) The functions W_{e_i} is quasiconvex at F if and only if $X(F, e_i, e_i) \geq 0$.

(c) If W_{e_j} is quasiconvex at F then $X(F, e_i, e_j) = W_{e_j}(F) + \kappa_{i\to j} - W_{e_i}(F)$.

Using the convexity together with $X(F, e_i, e_i) = 0$ we find the following useful characterizations.

Proposition 5.3
(a) The state (F, e_i) is a stable pure state if and only if there exists an $\varepsilon > 0$ such that $X(F, e_i, \widehat{c}) \geq 0$ for all $\widehat{c} \in \widehat{P}$ with $|\widehat{c}-e_i| < \varepsilon$.

(b) If $X(F, e_i, \widehat{c})$ is (one–sided) differentiable in $\widehat{c}$ at e_i, that is $X(F, e_i, \widehat{c}) = L \cdot (\widehat{c}-e_i) + o(|\widehat{c}-e_i|)$ for $\widehat{P} \ni \widehat{c} \to e_i$, then (F, e_i) is a stable pure state if and only if $L_j \geq L_i$ for all $j \neq i$.

Here the statement in (a) says that the most dangerous case is to insert a nucleus which has a relatively small volume fraction of transformed material. If this is impossible, then it is also impossible to insert a nucleus with a larger volume fraction. The statement in (b) has to be considered with care, as the assumed differentiability does not hold in general, see the example in Section 6. But if it holds, as for instance in the case $d = 1$, then it is very useful in the sense that we can establish stability by checking only the associated two–phase problems $X(F, e_i, (1-\theta)e_i + \theta e_j) = (L_j - L_i)\theta + o(\theta)$ for $0 < \theta \to 0$.

5.2 Stability of interfaces

We are now interested in the stability of smooth interfaces. We say that at x_0 there is a smooth interface if the interface is continuously differentiable in x_0 and the functions $c(x)$ and $F(x) = \nabla u(x)$ are continuous on each side of the interface such that the limits $(F^{\pm}, e^{\pm})$ from either side onto the interface exists.

As above, localization allows us to look at the piecewise linear case. The interface is given by $\Sigma_\nu = \{\, y \in I\!R^d \,:\, |y| < 1,\ y \cdot \nu = 0 \,\}$ and the unit ball decomposes into $B = B_\nu^- \cup \Sigma_\nu \cup B_\nu^+$ where $B_\nu^{\pm} = \{\, y \in B \,:\, \pm y \cdot \nu < 0 \,\}$. The state of the process in $B_\nu^{\pm}$ is given by $(e^{\pm}, F^{\pm})$; and we need compatibility conditions for the deformation and for the stresses:

$$F^+ - F^- = a \otimes \nu, \qquad [\partial_F W_{e^+}(F^+) - \partial_F W_{e^-}(F^-)]\nu = 0. \tag{5.1}$$

The first condition is needed to make $u(y) = F^{\pm} y$ continuous on Σ_ν, and the second is the force balance on the two sides of Σ_ν.

Definition 5.4
For $(F^-, F^+, e^-, e^+, \widehat{c}^-, \widehat{c}^+)$, where $(F^{\pm}, e^{\pm})$ satisfies (5.1), let $\widetilde{F}(y) = F^{\pm}$ and $\widetilde{c}(y) = e^{\pm}$ for $y \in B_\nu^{\pm}$ and define the function

$$Y_\nu(F^{\pm}, e^{\pm}, \widehat{c}^{\pm}) = \inf \Big\{ \fint_B \Big[W_{c(y)}(\widetilde{F}(y) + \nabla\phi(y)) + D(\widetilde{c}(y), c(y)) - W_{\widetilde{c}(y)}(\widetilde{F}(y)) \Big]\, \mathrm{d}y \ : \\ \phi \in \mathrm{W}_0^{1,p}(B),\ c \in \mathrm{L}^\infty(B, P),\ \fint_{B_\nu^{\pm}} c(y)\, \mathrm{d}y = \widehat{c}^{\pm} \Big\}$$

Then, the interface values $(F^{\pm}, e^{\pm})$ are **stable** *if $Y_\nu(F^{\pm}, e^{\pm}, \widehat{c}^{\pm}) \geq 0$ for all $\widehat{c}^{\pm} \in \widehat{P}$.*

Notice that the phase fractions $\widehat{c}^{\pm}$ are prescribed separately in $B_\nu^{\pm}$.

Theorem 5.5
(i) The mapping $(\widehat{c}^+, \widehat{c}^-) \mapsto Y(F^{\pm}, e^{\pm}, \widehat{c}^{\pm})$ is convex on $\widehat{P} \times \widehat{P}$.
(ii) We have the one–dimensional necessary condition

$$\int_{s=-1}^{1} \Big[W_{\overline{c}(s)}(\widetilde{F}(s\nu) + \varphi'(s) \otimes \nu) + D(\widetilde{c}(s\nu), \overline{c}(s)) - W_{\widetilde{c}(s\nu)}(\widetilde{F}(s\nu)) \Big]\, \mathrm{d}s \geq 0$$

for all $\overline{c} \in \mathrm{L}^\infty((-1,1), P)$ and $\varphi \in \mathrm{W}_0^{1,p}((-1,1))$.
(iii) With $T_0 = \partial_F W_{e^+}(F^+)\nu = \partial_F W_{e^-}(F^-)\nu$ we have the necessary condition

$$-D(e^+, e^-) \leq W_{e^-}(F^-) - W_{e^+}(F^+) + T_0 \cdot ([F^+ - F^-]\nu) \leq D(e^-, e^+). \tag{5.2}$$

In [Lev95, Lev97] the scalar quantity $\chi = W_{e^-}(F^-) - W_{e^+}(F^+) + T_0 \cdot ([F^+ - F^-]\nu)$ is called the driving force for the interface. As long as χ lies strictly between $-D(e^+, e^-)$ and $D(e^-, e^+)$ the interface cannot move in a time–continuous process since the dissipation plays the role of a threshold. If χ reaches the value $D(e^-, e^+)$ the interface can move such that phase e^+ grows, and analogously phase e^- will start to grow if $\chi = -D(e^+, e^-)$.

Proof: ad (i): The convexity follows as in Proposition 4.2, we only have to take care to separate the ball B in the definition of Y orthogonally to the interface.

ad (ii): We use special comparison functions of the form $c(y) = \overline{c}(s)$ and $\phi(y) = \delta\varphi(s/\delta)\psi(|y|)$ where $s = y\cdot\nu$ and $0<\delta\ll 1$. Integration in the transverse direction then gives the result.

ad (iii): We start from (ii) with the phase function $\overline{c}$ such that $\overline{c}(s) = e^-$ for $s\in(-1,\alpha)$ and $\overline{c}(s) = e^+$ for $s>\alpha$, where $|\alpha|\ll 1$ is assumed. Moreover, we let $\overline{f}(s) = 0$ for $s<0$ and $\overline{f}(s) = a$ for $s>0$ (see (5.1) for the definition of a) and $w(c,s,g) = W_c(F^-{+}g{\otimes}\nu)$ such that $W_c(\widetilde{F}(s\nu) + \varphi'(s){\otimes}\nu) = w(c, \overline{f}(s) + \varphi')$. Minimizing $\int_{-1}^1 w(\overline{c}(s), \overline{f}(s){+}\varphi'(s))\,\mathrm{d}s$ yields a unique solution φ satisfying $\partial_g w(\overline{c}(s), \overline{f}(s){+}\varphi(s)) = \sigma = \mathrm{const}$, where $\sigma\in\mathbb{R}^d$ is to be determined such that $\int_{-1}^1 \phi'(s)\,\mathrm{d}s = 0$. Denoting by $g = m_\pm(\sigma)$ the inverse function of $\sigma = \partial_g w(e^\pm, g)$ we arrive at the condition $(1{+}\alpha)m_-(\sigma) + (1{-}\alpha)m_+(\sigma) = \int_{-1}^1 \overline{f}(s)\,\mathrm{d}s = a$. Note that $\partial_g w(e^-,0) = \partial_g w(e^+,a) = \sigma_0$ implies that $\varphi\equiv 0$ is the unique solution for $\alpha = 0$. By the implicit function theorem we find locally a unique solution $\sigma = \overline{\sigma}(\alpha) = \sigma_0 + \alpha\sigma_1 + \mathcal{O}(\alpha^2)$, where $[D_\sigma m_-(\sigma_0) + D_\sigma m_+(\sigma_0)]\sigma_1 = m_+(\sigma_0) - m_-(\sigma_0) = a$. This defines the minimizers φ_α as a function of α and inserting this into the energy we arrive at

$$\begin{aligned}
&\int_{-1}^1 w(\overline{c}(s), \overline{f}(s){+}\varphi_\alpha'(s))\,\mathrm{d}s = \\
&w(e^-,0){+}w(e^+,a) + \alpha\,(w(e^-,0){-}w(e^+,a){+}\sigma_0\cdot[D_\sigma m_-(\sigma_0){+}D_\sigma m_+(\sigma_0)]\sigma_1) + \mathcal{O}(\alpha^2) = \\
&\int_{-1}^1 w(\widetilde{c}(s\nu), \overline{f}(s))\,\mathrm{d}s + \alpha\,(w(e^-,0){-}w(e^+,a){+}\sigma_0\cdot a) + \mathcal{O}(\alpha^2).
\end{aligned}$$

Inserting this into the stability criterion (ii) we obtain the desired two estimates in (5.2) by taking the limits $\alpha\to 0+$ and $\alpha\to 0-$, respectively (one–sided limits). QED

6 Explicit formulas in the case of quadratic energies

6.1 Relaxation for $d = 1$

In one space dimension the mixture function can be characterized more explicitly. Moreover, the the case that all W_{e_j} are quadratic functions the mixture function $\widehat{W_{\widehat{c}}}(F)$ can be given explicitly. The main point in one space dimension is that there are no compatibility restrictions: all gradients are scalars and hence rank–one connected. This leads to the fact that $\int_0^1 W_{c(x)}(F{+}\phi'(x))\,\mathrm{d}x$ only depends on $\widehat{c} = \int_0^1 c(x)\,\mathrm{d}x$. Using $\partial_F W_{c(x)}(F{+}\phi'(x)) = \sigma + \mathrm{const}$ it is not difficult to see that the Legendre transform is the right tools to calculate $\widehat{W_{\widehat{c}}}(F)$. The Legendre transform $\mathcal{L}W$ of a convex function W is given by $(\mathcal{L}W)(\sigma) = \inf\{\,\sigma F - W(F)\ :\ F\in\mathbb{R}\,\}$. and we obtain the formula

$$\widehat{W_{\widehat{c}}}(F) = \mathcal{L}^{-1}\Big(\sum_{j=1}^n (\widehat{c}\cdot e_j)\mathcal{L}W_{e_j}\Big).$$

We refer to [Mie98] for more details.

In the case of quadratic case with

$$W_{e_i}(F) = \frac{1}{H_i}(F{-}A_i)^2{+}B_i \quad \text{with } H_i>0 \tag{6.1}$$

we find the expression

$$\widehat{W_{\widehat{c}}}(F) = \frac{(F - A\cdot\widehat{c})^2}{H\cdot\widehat{c}} + B\cdot\widehat{c}. \tag{6.2}$$

Here we use the notation $A = (A_1,\ldots,A_n)^T$ and similarly for $B, H\in\mathbb{R}^n$.

Remark 6.1 It is important to realize that in general the solution of (RIP) is not unique. This is seen most simple in the case $d = 1$ and quadratic energy densities $W_{e_i}(F) = (F-A_i)^2/H_i + B_i$. Consider $\widehat{a} \equiv 0$, $V = \{ u \in \mathrm{W}^{1,2}((0,\ell)) \ : \ u(0) = 0, u(1) = \ell\xi \}$, and $G = 0$, then $\widehat{I}(\widehat{c}) = \widehat{W}_{\widehat{b}}(\xi)$ for all $\widehat{c} \in \mathrm{L}^\infty(\Omega, \widehat{P})$ with $⨍_0^\ell \widehat{c}(x)\,\mathrm{d}x = \widehat{b}$. Thus, the infimum of $\widehat{I}(\cdot) + \widehat{\mathcal{D}}(\widehat{a}, \cdot)$ over $\mathrm{L}^\infty(\Omega, \widehat{P})$ is attained for each $\widehat{c}$ such that $⨍_0^\ell \widehat{c}(x)\,\mathrm{d}x = \widehat{c}^*$, where $\widehat{c}^*$ is the minimizer of $\widehat{W}_{\cdot}(\xi)+\widehat{D}(\widehat{a},\cdot)$ over $\widehat{P}$. Thus we obtain an uncountable number of solutions, e.g. the constant microstructure $\widehat{c}(x) = \widehat{c}^*$ for all x or the solution $\widehat{c}(x) = e_j$ for $x \in [\ell(\theta_1+\ldots+\theta_j), \ell(\theta_1+\ldots+\theta_{j+1})$, where $\widehat{c}^* = \sum_1^n \theta_j e_j$.

More delicate nonuniqueness results in higher space dimensions are discussed in [GrK95].

Moreover, the mixture theory in dimension $d = 1$ is somehow artificial as it is possible to show that even the nonrelaxed problem (IP) always has a solution as long as the external loading functional $\langle G(t), \cdot \rangle$ is given in the form $\int_{x_0}^{x_1} f(t,x)u(x)\,\mathrm{d}x + \lambda(t)u(t,x_2)$, see [Mie98].

For one–dimensional linearized elasticity (see (6.1)) The function X, which determines the stability of pure phases can be calculated explicitly using the mixture function $\widehat{W}_{\widehat{c}}(F)$ from (6.2). We obtain $X(F, e_i, \widehat{c}) = \frac{(F-A\cdot\widehat{c})^2}{H\cdot\widehat{c}} + B\cdot\widehat{c} + \overline{D}\cdot\widehat{c} - W_{e_i}(F)$. Clearly, Proposition 5.3(b) is applicable and a simple calculation gives

$$L_j = \partial_{\widehat{c}\cdot e_j} X(F, e_i, e_i) = \tfrac{1}{H_i^2}[2(A_i-F)A_j H_i - (A_i-F)^2 H_j] + B_j + \kappa_{i\to j}.$$

After some rearrangements the conditions $L_j \geq L_i$ take the following form.

Proposition 6.2
Let W_{e_i} be of the form (6.1). *Then, $X(F, e_i, \widehat{c}) \geq 0$ for all $\widehat{c} \in \widehat{P}$ if and only if*

$$W_{e_j}(F) + \kappa_{i\to j} \geq W_{e_i}(F) + \frac{1}{H_i^2 H_j}\left(A_i H_j - A_j H_i + F(H_i-H_j)\right)^2 \quad \text{for } j \neq i.$$

In the case $H_j = H$ for $j = 1, \ldots, n$, this condition simplifies to

$$W_{e_j}(F) + \kappa_{i\to j} \geq W_{e_i}(F) + \tfrac{(A_j-A_i)^2}{H} \quad \text{for all } j \neq i.$$

This result is stronger than imposing $X(F, e_i, e_j) = W_{e_j}(F) + \kappa_{i\to j} - W_{e_i}(F) \geq 0$ for $j \neq i$ because of the additional quadratic term. This relates to the fact, that $X(F, e_i, e_j) > 0$ says that a PT of the *whole* domain B is energetically not favorable, however the local condition $L_j \geq L_i$ says that insertion of infinitesimal small regions with phase e_j is not favorable.

6.2 A two–phase problem with $d \geq 2$

Using results of [Kha67, Roi67, Kha83, Koh91] we show how the higher–dimensional problem can be approached in the case of linearized elasticity. Strict results are available only for the case of two phases.

$$W_{e_i}(F) = \tfrac{1}{2}\langle \mathbf{C}(E-A_i), E-A_i \rangle + B_i \quad \text{where } E = \tfrac{1}{2}(F+F^T)-I. \tag{6.3}$$

Here $E, A_i \in S(d) = \{ M \in I\!R^{d\times d} \ : \ M = M^T \}$, the set of symmetric matrices, where we continue to use the scalar product $\langle E, A\rangle = \sum_{i,j} E_{ij}A_{ji}$. The symmetric tensor E is the linearized strain, and the elasticity tensor $\mathbf{C}$ is assumed to be positive definite, that is

$$\langle \mathbf{C}E, E\rangle = \sum_{i,j,k,l=1}^{d} \mathbf{C}_{ijkl}E_{ij}E_{kl} \geq \alpha \|E\|^2 \quad \text{for } E \in S(d)$$

with $\alpha > 0$. The following result is due to R.V. Kohn, cf. [Koh91].

Theorem 6.3
Consider W_{e_i} as in (6.3) and let $\widehat{c}_\theta = \theta e_1 + (1-\theta)e_2$ for $\widehat{\theta} \in [0,1]$. Then, the mixture function is given by

$$\widehat{W}_{\widehat{c}_\theta}(F) = \theta W_{e_1}(F) + (1-\theta)W_{e_2}(F) - \theta(1-\theta)\beta$$

where β is determined from $\mathbf{C}$ and $A_1 - A_2$ via $\beta = \frac{1}{2}\max\{ \|P_\xi(\mathbf{C}^{1/2}(A_1-A_2)\|^2 \ : \ \xi \in I\!R^d, \ |\xi| = 1\}$ where P_ξ is the orthogonal projection in $(S(d), \langle\cdot,\cdot\rangle)$ onto the space $\{ \mathbf{C}^{1/2}(\xi\otimes v + v\otimes\xi) \ : \ v \in I\!R^d \}$.

Thus, the mixture function always lies below the simple affine combination. A somewhat simpler formula for β, which avoids the square root $\mathbf{C}^{1/2}$, is

$$\beta = \max\left\{ \frac{\langle \mathbf{C}(A_1-A_2), S\rangle^2}{2\langle \mathbf{C}S, S\rangle} \ : \ S = \xi\otimes v + v\otimes\xi, \ \xi, v \in I\!R^d \setminus \{0\} \right\}. \tag{6.4}$$

To have a closer relationship to the analysis for the case $d = 1$ with $n = 2$ we use the form

$$\begin{aligned}\widehat{W}_{\widehat{c}_\theta}(F) &= \tfrac{1}{2}\langle \mathbf{C}(E-\theta A_1-(1-\theta)A_2), (E-\theta A_1-(1-\theta)A_2)\rangle + \theta B_1 + (1-\theta)B_2 + \theta(1-\theta)[\gamma-\beta],\\ &\text{where } \gamma = \tfrac{1}{2}\langle \mathbf{C}(A_1-A_2), A_1-A_2\rangle \geq \beta,\end{aligned} \tag{6.5}$$

which follows by simple calculations using the quadratic form of W_{e_i}. Clearly we find $\gamma = \beta$ if and only if $A_1 - A_2$ can be written in the form $k\otimes v + v\otimes k$ for some $k, v \in I\!R^d$. This is always the case for $d = 1$ and thus, we have complete agreement with (6.2) for the special case $H_1 = H_2 = 2/\mathbf{C} > 0$. Of course, (6.2) provides the generalization to general linear problems with $n \geq 2$ phases and different elastic constants H_j.

We want to apply this formula to the stability of pure phases in the higher dimensional case. Using the above notation we have $X(F, e_1, \theta e_1 + (1-\theta)e_2) = (1-\theta)[W_{e_2}(F) + D(e_1, e_2) - W_{e_1}(F) - \theta\beta]$. Like in the one dimensional case we see that it is sufficient to check the case $\theta \approx 1$.

Corollary 6.4
Let W_{e_1}, W_{e_2}, and β as in Theorem 6.3, then (F, e_1) is stable if and only if $W_{e_2}(F) + \kappa_{1\to 2} \geq W_{e_1}(F) + \beta$.

For isotropic linearized elasticity we give the following examples for β as a function of $\mathbf{C}$ and $A_1 - A_2$.

Lemma 6.5
Let $\mathbf{C}(E) = \lambda\langle E, I\rangle I + 2\mu E$. *Then,*
(a) for $A_1{-}A_2 = \eta I{+}\delta\, e_1{\otimes}e_1$ *we have*

$$\beta = \frac{[\eta(d\lambda{+}2\mu) + \delta(\lambda{+}2\mu)]^2}{2(\lambda{+}2\mu)} \quad \text{and } \gamma = [d(d\lambda{+}2\mu)\eta^2 + 2(d\lambda{+}2\mu)\eta\delta + (\lambda{+}2\mu)\delta^2]/2,$$

(b) and for $A_1{-}A_2 = \eta(e_1\otimes e_2 + e_2\otimes e_1)$ *we have* $\beta = \gamma = 2\mu\eta^2$.

Proof: For $S = \xi{\otimes}v + v{\otimes}\xi$ we find $\langle\mathbf{C}S, S\rangle = 4[(\lambda{+}\mu)(\xi\cdot v)^2 + \mu|\xi|^2|v|^2]$.

ad (a) Let $T = \eta I{+}\delta\, e_1{\otimes}e_1$, then $\mathbf{C}(T) = \lambda(d\eta{+}\delta)I + 2\mu(\delta\, e_1{\otimes}e_1{+}\eta I)$. Evaluating $\langle C(T), T\rangle$ gives γ. Moreover, $\langle C(T), S\rangle = 2\lambda(d\eta{+}\delta)\xi\cdot v + 4\mu(\eta\xi\cdot v{+}\delta\xi_1 v_1)$. Thus, the maximum is achieved for $\xi = v = e_1$.

ad (b) With $T = e_1{\otimes}e_2{+}e_2{\otimes}e_1$ we find $\langle\mathbf{C}(T), S\rangle = 4\mu(\xi_1v_2{+}\xi_2v_1)$ and the maximum is achieved for $\xi = e_1$ and $v = e_2$. QED

For more than two different phases only partial results are known, see [Koh91, Sect. 8]. However, they are strong enough to show that the mixture function $\widehat{W}_{\widehat{c}}(F)$ is in general not differentiable in $\widehat{c}$. The following result is a consequence of [Koh91], see Prop. 8.2 and the example in (8.26) and (8.27). The result is a generalization of the fact that $\gamma = \beta$ in (6.5).

Theorem 6.6
Assume that $W_{e_j}(F)$, $j = 1, 2, 3$, *are given as in* (6.3). *Moreover, assume that there exists vectors* $k_i, v_i \in \mathbb{R}^d$, $i = 1, 2$, *and a* $\rho \in (0, 1)$ *such that the compatibility conditions*

$$A_1 - A_2 = k_1{\otimes}v_1 + v_1{\otimes}k_1 \quad \text{and } A_3 - [\rho A_1{+}(1{-}\rho)A_2] = k_2{\otimes}v_2 + v_2{\otimes}k_2$$

hold. Then, for $\widehat{c}_\theta = \theta[\rho e_1{+}(1{-}\rho)e_2] + (1{-}\theta)e_3$ *with* $\theta \in [0, 1]$ *the formula*

$$\widehat{W}_{\widehat{c}_\theta}(F) = \tfrac{1}{2}\langle\mathbf{C}(E{-}\widehat{A}_\theta), E{-}\widehat{A}_\theta\rangle + \widehat{c}_\theta\cdot B, \quad \text{where } \widehat{A}_\theta = \textstyle\sum_{k=1}^3(\widehat{c}_\theta\cdot e_k)A_k, \tag{6.6}$$

holds.

The proof again relies on the construction of a microstructure which in this case is sequentially laminated.

We apply this result in the case $d = 2$ with $\mathbf{C}E = E$ (that is $\lambda = 0$ and $\mu = 1/2$ in Lemma 6.5), $B_k = 0$, and the matrices

$$A_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad A_3 = 0.$$

The assumptions of Theorem 6.6 are satisfied with $\rho = 1/2$ and (6.6) gives with $\widehat{c}_\theta = \frac{\theta}{2}(e_1{+}e_2){+}(1{-}\theta)e_3$ and $\widehat{A}_\theta = \theta\, e_1{\otimes}e_1$ the relation $\widehat{W}_{\widehat{c}_\theta}(F) = \frac{1}{2}\|E{-}\widehat{A}_\theta\|^2$. Comparing this result for a three–phase mixture with the results for the two–phase mixtures of Theorem 6.3 we obtain for $F = 0$ the formulae

$$\widehat{W}_{\widehat{c}_\theta}(0) = \theta^2/2, \quad \widehat{W}_{\theta e_1+(1-\theta)e_3}(0) = \widehat{W}_{\theta e_2+(1-\theta)e_3}(0) = (\theta{+}\theta^2)/2$$

which clearly shows that $\widehat{W}_{\widehat{c}_\theta}(0)$ cannot be differentiable at $\widehat{c} = e_3$.

6.3 Explicit calculation of $\Psi(\widehat{a}, F)$

We show that for the example of linearized elasticity in dimension $d \geq 1$ with two phases the functions $\Psi(\widehat{a}, F)$ and $\widehat{C}(\widehat{a}, F)$ can be given explicitly. Thus, it is possible to solve the relaxed incremental problem in the form (RIP)' numerically in an easy way if a suitable finite element code for nonlinear variational problems is available.

The nice feature is that the functions $\widehat{\Psi}(\widehat{a}, F)$ and $\widehat{C}(\widehat{a}, F)$ (see (4.8)) are determined solely from the family $(W_{e_j}(F))_{j=1,\dots,n}$. In principle, they can be calculated before starting to consider (RIP)' and then it remains to solve the minimization problem $\widehat{\mathcal{E}}(t_k, \widehat{c}_{k-1}, u_k) = \inf\{\, \mathcal{E}(t_k, \widehat{c}_{k-1}, v) \;:\; v \in V \,\}$ where $\widehat{\mathcal{E}}(t, \widehat{a}, v) = \int_\Omega \widehat{\Psi}(\widehat{a}(x), \nabla v(x))\,\mathrm{d}x - \langle G(t), v\rangle$.

Here we want to show that for certain cases the functions $\widehat{\Psi}$ and $\widehat{C}$ can be calculated explicitly. One possible case is the one–dimensional case with arbitrarily many phases (i.e. $d = 1$ and $n \geq 2$) with quadratic energies as in (6.1). However, here we restrict to the more relevant higher-dimensional case with two cases which was treated in the previous section. Using the above notations toghether with the variables $\theta, \vartheta \in [0, 1]$ in

$$\widehat{a} = \vartheta e_1 + (1{-}\vartheta)e_2 \text{ and } \widehat{c} = \theta e_1 + (1{-}\theta)e_2$$

and the dissipation $\kappa_{1\to2} = \kappa_{2\to1} = \kappa > 0$ we arrive at

$$\begin{array}{rcl} \widehat{\Psi}(\vartheta, F) &=& \frac{1}{2}\langle \mathbf{C}(E{-}A_2), E{-}A_2\rangle{+}B_2 + 2\beta\mathcal{G}_{\kappa/(2\beta)}(\vartheta, \langle E, \widetilde{A}\rangle{+}\alpha), \\ \Theta(\vartheta, F) &=& \Theta_{\kappa/(2\beta)}(\vartheta, \langle E, \widetilde{A}\rangle{+}\alpha), \end{array}$$

with β from (6.4), $\alpha = \frac{1}{4\beta}(\langle \mathbf{C}A_1, A_1\rangle{-}\langle \mathbf{C}A_2, A_2\rangle{+}2B_1{-}2B_2){-}1/2$ and $\widetilde{A} = \frac{1}{2\beta}\mathbf{C}(A_2{-}A_1)$. Here we have used the formula in Theorem 6.3 and the expressions in the appendix applied to $\widehat{\Psi}(\vartheta, F) = \inf_{\theta\in[0,1]} \widehat{W}_{\theta e_1+(1-\theta)e_2} + \kappa|\vartheta{-}\theta|$.

In general the function $F \mapsto \widehat{\Psi}(\vartheta, F)$ is not necessarily convex, but only quasiconvex. We show this by reducing the general formula to the special case with $B_1 = B_2 = 0$, $A_2 = 0$, $A_1 = \eta I$, and $\mathbf{C}E = E$, that is linearized elasticity with Lamé constants $\lambda = 0$ and $\mu = 1/2$. We obtain $\beta = \eta^2/2$, $\alpha = (d{-}1)/2$, and $\widetilde{A} = -(1/\eta)I$ and thus arrive at

$$\begin{array}{rcl} \widehat{\Psi}(\vartheta, F) &=& \frac{1}{2}\|E\|^2 + \eta^2\mathcal{G}_{\kappa/\eta^2}(\vartheta, (d{-}1)/2{-}\langle E, I\rangle/\eta), \\ \Theta(\vartheta, F) &=& \Theta_{\kappa/\eta^2}(\vartheta, (d{-}1)/2{-}\langle E, I\rangle/\eta). \end{array}$$

Since we have chosen a PT which is purely volumetric ($A_1{-}A_2 = \eta I$), the nonlinearity of the problem is only due to the trace $\langle E, I\rangle$ of E. Evaluating $\widehat{\Psi}(\vartheta, \cdot)$ at $F_\tau = (1{+}\tau)I$ we find

$$\widehat{\Psi}(\vartheta, F_\tau) = d\tau^2/2 + \eta^2\mathcal{G}_{\kappa/\eta^2}(\vartheta, (d{-}1)/2{-}d\tau/\eta). \tag{6.7}$$

Clearly this function is nonconvex as from the explicit form of $\mathcal{G}$ given in the appendix we find that the second derivative of $\tau \mapsto \widehat{\Psi}(\vartheta, F_\tau)$ attains exactly the values d and $-2d$. The negative second derivative occurs exactly on those intervals where the new volume fraction $\theta = \Theta_{\kappa/\eta^2}(\vartheta, (d{-}1)/2 - d\tau/\eta)$ is not equal to either $0, \vartheta$, or 1.

6.4 Necessity of microstructure

Finally we want to give the simplest example which shows that (IP) in general does not have a solution while (RIP) is solvable with a solution not lying $\mathrm{L}^\infty(\Omega, \widehat{P}) \setminus (\mathrm{L}^\infty(\Omega, P))$.

It is fairly easy to show that (RIP) has a solution with microstructure. In fact, using Proposition 4.2 we know that $\widehat{\Psi}(\widehat{a}, \cdot)$ is quasiconvex. Hence, prescribing homogeneous boundary data $u(x) = Fx$ on $\partial\Omega$, we immediately conclude that $u : x \mapsto Fx$ is a global minimizer. If F is chosen such that $\widehat{c} = \widehat{C}(\widehat{a}, F)$ lies in $\widehat{P} \setminus P$, then this corresponds to a solution with microstructure.

To prove that (IP) has no solution it suffices to show that the given solution of (RIP) is unique. However, in general (RIP) might have several solutions as was pointed out in [GrK95], some having microstructure and others having no microstructure. The problem of nonuniqueness already occurs in space dimension $d = 1$ (cf. Remark 6.1) where in fact (IP) always is solvable and (RIP) might have microstructure solutions as well, see [Mie98].

The following example gives the desired uniqueness result in the framework of linearized elasticity with two phases whose transformations strains are rank–one connected. Again consider the situation of Section 6.2 with $\mathbf{C}E = E$, $B_1 = B_2 = 0$, and $A_1 = -A_2 = e_1 \otimes e_1$. The initial phase distribution is $c_0(x) = e_1$ (that is $\vartheta \equiv 1$) on the domain $\Omega = (0,1)^2 \subset I\!R^2$ with $V = \mathrm{W}_0^{1,2}(\Omega)$ (that is $u|_{\partial\Omega} = 0$). By the definition of the mixture function we know that $\widehat{I}(\widehat{c}) \geq \widehat{W}_{\widehat{b}}(0)$ for all $\widehat{c} \in \mathrm{L}^\infty(\Omega, \widehat{P})$ with $⨍_\Omega \widehat{c}(x)\,\mathrm{d}x = \widehat{b}$. With $\widehat{b} = \theta e_1 + (1-\theta)e_2$ and we conclude

$$\widehat{J}(c_0, \widehat{c}) = \widehat{I}(\widehat{c}) + \widehat{\mathcal{D}}(\widehat{a}, \widehat{c}) \geq (1-2\theta)^2/2 + \kappa_{1\to2}(1-\theta)$$

where we have used (6.5) together with Lemma 6.5(b).

Now assuming $\kappa = \kappa_{1\to2} < 2$ we find that the infimum of $\widehat{J}(e_1, \cdot)$ is larger or equal to $\kappa(\kappa-4)/8$ which is the value for $\theta^* = (\kappa+2)/4$. It is easy to see that this infimum is attained in (RIP) by the solution $(\widehat{c}, u) \equiv (\widehat{c}^*, 0)$ with $\widehat{c}^* = \theta^* e_1 + (1-\theta^*)e_2$.

It remains to be shown that this infimum is not attained $\mathrm{L}^\infty(\Omega, P)$, which means that (IP) has no solution. We summarize this in

Proposition 6.7
Assume $\kappa \in (0,4)$ then for $J(e_1, c) = I(c) + \mathcal{D}(e_1, c)$ we have $J(e_1, c) > \inf\{\, J(e_1, a) \,:\, a \in \mathrm{L}^\infty(\Omega, P)\,\} = \kappa(\kappa-4)/8$ for all $c \in \mathrm{L}^\infty(\Omega, P)$.

Proof: To simplify the notation write $K(\theta) = J(e_1, c_\theta)$ with $c_\theta(x) = \theta e_1 + (1-\theta)e_2$ where $\theta(x) \in \{0, 1\}$. We have

$$K(\theta) = \inf\{\, \widetilde{E}(\theta, u) \,:\, u \in \mathrm{W}_0^{1,2}((0,1)^2)\,\} \text{ with}$$
$$\widetilde{E}(\theta, u) = \textstyle\int_{(0,1)^2} [(\partial_{x_1} u_1 + 1 - 2\theta)^2 + (\partial_{x_2} u_1)^2 + (\partial_{x_1} u_2)^2 + (\partial_{x_2} u_2)^2 + \kappa(1-\theta)]\,\mathrm{d}x.$$

We first show that the infimum must be smaller or equal to $\kappa(\kappa-4)/8$. Take $\theta^* = (\kappa+2)/4$ and define $(y(s), z(s)) = (1, 2(1-\theta^*)s)$ for $s \in [0, \theta^*)$ and $(y(s), z(s)) = (0, 2\theta^*(1-s)$ for $s \in [\theta^*, 1)$ as periodic functions on $I\!R$ via $(y(s), z(s)) = (y(s+1), z(s+1))$. For $m \in I\!N$ define $\theta_m(x) = y(mx_1)$ and $u_m(x) = (\min\{1, mx_2(1-x_2)\} z(mx_1), 0)^T$. From $K(\theta_m) \leq \widetilde{E}(\theta_m, u_m)$ we find

$$K(\theta_m) \leq \tfrac{1}{2}[\theta^*(2(1-\theta^*) - 1)^2 + (1-\theta^*)[(-2\theta^*+1)^2) + \kappa]] + \mathcal{O}(1/m)_{m\to\infty}$$

which gives the desired estimate $\inf K(\cdot) \leq \kappa(\kappa-4)/8$.

The opposite conclusion is obtained as follows. The one–dimensional theory applied to every $x_2 \in (0,1)$ gives $\int_0^1 [(\partial_{x_1} u_1 + 1 - 2\theta)^2 + \kappa(1-\theta)]\,\mathrm{d}x_1 \geq \kappa(\kappa-4)/8$. Integration over $x_2 \in (0,1)$ gives $J(e_1, c_\theta) \geq \kappa(\kappa-4)/8 + \int_{(0,1)^2} (\partial_{x_2} u_1)^2\,\mathrm{d}x$. Thus, if the value $\kappa(\kappa-4)/8$ would be achieved, then $\partial_{x_2} u_2 = 0$ together with the boundary conditions $u = 0$ would imply $u \equiv 0$. But this is impossible, since $\widetilde{E}(\theta, 0) > \kappa(\kappa-4)/8$. QED

A A piecewise quadratic minimization problem

For $\rho > 0$ we consider the function

$$f_\rho(b, \vartheta, \theta) = \theta^2/2 - b\theta + \rho|\theta - \vartheta|$$

with $\vartheta, \theta \in [0,1]$, and $b \in I\!R$. Using the piecewise quadratic form of f as a function of θ it is possible to give explicit expressions for

$$\mathcal{G}_\rho(\vartheta, b) = \min\{\, f(b, \rho, \vartheta, \theta) \;:\; \theta \in [0,1] \,\} \quad \text{and } \Theta_\rho(\vartheta, b) = \arg\min f_\rho(b, \vartheta, \cdot).$$

In fact, we have

$$(\mathcal{G}_\rho(\vartheta, b), \Theta_\rho(\vartheta, b)) = \begin{cases} (\rho\vartheta\,, 0) & \text{for } b \le -\rho, \\ (\rho\vartheta - (b+\rho)^2/2\,, b+\rho) & \text{for } b \in [-\rho, \vartheta-\rho], \\ (\vartheta^2/2 - b\vartheta\,, \vartheta) & \text{for } b \in [\vartheta-\rho, \vartheta+\rho], \\ (-(b-\rho)^2/2 - \rho\vartheta\,, b-\rho) & \text{for } b \in [\vartheta+\rho, 1+\rho], \\ (1/2 - b + \rho(1-\vartheta)\,, 1) & \text{for } b \ge 1+\rho. \end{cases}$$

We note that $\partial_b \mathcal{G}_\rho(\vartheta, b) = -\Theta_\rho(\vartheta, b)$ and that Θ_ρ is increasing in b. This implies that $\mathcal{G}_\rho$ is a concave function in b.

B Some results on Banach–space valued functions of bounded variation

Definition B.1
Let X be a Banach space, then the set

$$BV([0,T], X) = \{ u \in L^1([0,T], X) \mid \|u\|_{BV} < \infty \}$$

is denoted by the space of functions of bounded variation with values in X. The norm $\|\cdot\|_{BV}$ is defined by

$$\begin{aligned} \|u\|_{BV} \;=\; & \sup\Big\{ \textstyle\int_0^T \langle u(t), \dot\varphi(t)\rangle \, \mathrm{d}t \;:\; \varphi \in C_c^1([0,T], X^*), \; \max_{t\in[0,T]} \|\varphi(t)\|_{X^*} \le 1 \Big\} \\ & + \|f\|_{L^1([0,T],X)}. \end{aligned}$$

The formula for $\|\cdot\|_{BV}$ shows that every $u \in BV([0,T], X)$ defines a bounded functional $\dot u$ on $C([0,T], X^*)$, but if X is not reflexive then the dual space $C([0,T], X^*)^*$ is larger than $BV([0,T], X)$. An important property of BV-functions is that they are continuous except on an at most countable set and that at every discontinuity point the left and the right–hand side limits exist.

Proposition B.2
Let $u \in BV([0,T], X)$ then for every $t \in [0,T]$ there exist $u_-(t), u_+(t) \in X$ so that for every sequence $t_\pm^n \to t$ as $n \to \infty$ consisting of Lebesgue points of u which satisfies $\pm(t - t_\pm^n) < 0$, the identity $\lim_{n\to\infty} u(t_\pm^n) = u_\pm(t)$ holds. The set of discontinuity points $t \in [0,T]$, for which $u_-(t) \ne u_+(t)$ holds, is at most countable.

Proof: We first prove that $u(t_n^-)$ is a Cauchy sequence. If this were not the case there would exist a positive number ε and two subsequences $(u(t_{\ell_n}^-))_{n\in I\!N}$ and $(u(t_{m_n}^-))_{n\in I\!N}$ so that $\|u(t_{\ell_n}^-)-u(t_{m_n}^-)\| \geq \varepsilon$. Since t_n^- is smaller than t we can extract a further subsequence (not relabeled) so that $t_{\ell_1}^- < t_{m_1}^- < t_{\ell_2}^- \ldots$. Using the hypothesis that $(t_n^-)_{n\in I\!N}$ consists of Lebesgue points of u we find that there exists a sequence of Lipschitz continuous mappings $v_k : [0,T] \to X^*$ satisfying $\max_{t\in[0,t]} \|v_k(t)\|_{X^*} \leq 1$ so that $\int_0^T \langle u, \dot{v}_k\rangle \;\mathrm{d}t \geq \frac{k}{2}\varepsilon$. For example take

$$v_k = \begin{cases} \alpha_i(t - t_{\ell_i} + \varepsilon(k))/(2\varepsilon(k)), & t \in [t_{\ell_i} - \varepsilon(k), t_{\ell_i} + \varepsilon(k)), \\ \alpha_i, & t \in [t_{\ell_i} + \varepsilon(k), t_{m_i} - \varepsilon(k)], \\ \alpha_i(t_{m_i} + \varepsilon(k) - t)/(2\varepsilon(k)), & t \in (t_{m_i} - \varepsilon(k), t_{m_i} + \varepsilon(k)], \\ 0, & \text{else} \end{cases}$$

for $i = 1 \ldots k$ and a suitably chosen $\varepsilon(k) > 0$. The points $\alpha_i \in X^*$ are chosen in such a way that $\langle \alpha_i, u(t_{\ell_i}) - u(t_{m_i})\rangle \geq \varepsilon$ holds. This is a contradiction to $|\!|\!| u |\!|\!|_{BV} < \infty$.

For a discontinuity point $t \in [0,T]$ let $h_u(t)$ be the jump height:

$$h_u(t) = \sup\{\, \|u(t_n^+) - u(t_n^-)\|_X \;:\; t_n^\pm \to t,\; t_n^\pm \text{ are Lebesgue points of } u.\}$$

Using the same argumentation as above on finds that $\sum_{t\in[0,T]} h_u(t) \leq |\!|\!| u |\!|\!|_{BV}$. This implies that h_u is nonzero for a at most countable subset of $[0,T]$. QED

The above proposition states that each element $u \in BV([0,T],X)$ can be identified with u_+ since each t where $u_-(t) = u_+(t)$ holds is automatically a Lebesgue point. Hence, assuming that $u = u_+$ we have the equivalent norm

$$|\!|\!| u |\!|\!|_{BV} = \|u(0)\| + \sup\{\sum_{j=1}^m \|u(t_j)-u(t_{j-1})\| \;:\; m \in I\!N,\; 0 = t_0 < t_1 < \ldots < t_m = T\,\}$$

We denote by $C_c^\infty(\Omega, I\!R^n)$ the space of test functions which are infinitely often differentiable and have compact support. In the following the target space is $I\!R^n$ if no specification is made. The dual space $C_c^\infty(\Omega)'$ is referred to as the space of distributions. The set of phase mixtures

$$\mathcal{S} = \{c \in C_c^\infty(\Omega)' \;|c \geq 0 \text{ and } \textstyle\sum_{i=1}^n c_i = 1\}$$

is a simplex in $C_c^\infty(\Omega)'$. $\mathcal{S}$ consists of bounded functions thus the inclusion $\mathcal{S} \subset L^1(\Omega) \subset W^{-1,1}(\Omega)$ holds. The topologies on $L^1(\Omega)$ and $W^{-1,1}(\Omega)$ are finer than the topology on $C_c^\infty(\Omega)'$, $\mathcal{S}$ is an intersection of closed sets in $C_c^\infty(\Omega)'$, therefore $\mathcal{S}$ is a closed subset of $L^1(\Omega)$ and $W^{-1,1}(\Omega)$.

Lemma B.3
For every $1 \leq p \leq \infty$ the norm $\|\cdot\|_{W^{-1,1}}$ metrizes the $L^p(\Omega)$–weak convergence (weak* if $p = \infty$) and the $W^{-1,1}(\Omega)$–weak* convergence on $\mathcal{S}$.

Proof: Let $f_n, f \in \mathcal{S}$, $\|f - f_n\|_{W^{-1,1}(\Omega)} \to 0$ as $n \to \infty$ and $g \in L^1(\Omega)$. Choose $g_\varepsilon \in W_0^{1,\infty}(\Omega)$ so that $\|g - g_\varepsilon\|_{L^1(\Omega)} \leq \varepsilon$. Now

$$\begin{aligned} |\textstyle\int_\Omega g \cdot (f_n - f) \;\mathrm{d}x| &\leq |\textstyle\int_\Omega (g - g_\varepsilon)\cdot(f - f_n) \;\mathrm{d}x| + |\textstyle\int_\Omega g_\varepsilon(f_n - f) \;\mathrm{d}x| \\ &\leq 2\varepsilon\|\mathcal{S}\|_{L^\infty(\Omega)} + \|g_\varepsilon\|_{W_0^{1,\infty}(\Omega)} \|f_n - f\|_{W^{-1,1}(\Omega)}. \end{aligned}$$

Using the fact that $\mathcal{S}$ is a bounded subset of $L^\infty(\Omega)$ and $\varepsilon > 0$ can be chosen arbitrarily small and taking the limit $n \to \infty$, one sees that $f_n - f$ converges weakly to 0 in $L^p(\Omega)$ and $W^{-1,1}(\Omega)$.

Now let $p > 1$ and $f_n - f$ converge weakly to 0 in $L^p(\Omega)$ (weak* if $p = \infty$) which is equivalent to the weak* convergence to 0 in $W^{-1,1}(\Omega)$. Assume that there exists $\varepsilon > 0$ and a sequence g_n so that $\|g_n\|_{W_0^{1\infty}(\Omega)} \leq 1$ and $\int_\Omega g_n \cdot (f_n - f)\, dx \geq \varepsilon$ for every n. Due to the compactness of the imbedding of $W_0^{1,\infty}(\Omega)$ into $L^{p'}(\Omega)$, $\frac{1}{p} + \frac{1}{p'} = 1$, for $1 < p \leq \infty$ there exists a subsequence g_n (not relabeled) which converges in $L^{p'}(\Omega)$ to some function g in $W_0^{1,\infty}(\Omega)$. Thus

$$\lim_{n\to\infty} \int_\Omega g_n \cdot (f_n - f)\, dx = \lim_{n\to\infty} \int_\Omega (g_n - g)(f_n - f)\, dx + \lim_{n\to\infty} \int_\Omega g \cdot (f_n - f)\, dx = 0$$

because of the boundedness of $\mathcal{S}$ in $L^p(\Omega)$. This is a contradiction, therefore we have that $\lim_{n\to\infty} \|f - f_n\|_{W^{-1,1}(\Omega)} = 0$.

If $p = 1$ use the density of $L^\infty(\Omega)$ in $L^q(\Omega)$ for $1 < q \leq \infty$ to see that the weak convergence also holds in $L^q(\Omega)$ and the preceding argumentation can be applied. QED

For the existence proof of time continuous functions which are limits of the incremental solutions, we use the result that the functions with bounded variation are under certain assumptions compactly imbedded into the set of integrable functions.

Theorem B.4
The set $\mathcal{T} = \{\, u \in BV([0,T], L^1(\Omega)) \;:\; \|u\|_{BV} \leq 1,\; u(t) \in \mathcal{S}$ *for a.e.* $t \in [0,T] \,\}$ *is a compact subset of* $L^1([0,T], W^{-1,1}(\Omega))$.

Proof: The relatively compact subsets F of $L^1([0,T], W^{-1,1}(\Omega))$ can be characterized by two conditions [Sim87, Theorem 1]:

1. $\left\{ \int_{t_1}^{t_2} u(t)\, dt \;\middle|\; u \in F,\ 0 < t_1 < t_2 < T \right\}$ is relatively compact in $W^{-1,1}(\Omega)$,
2. $\lim_{h\to 0} \sup\{ \int_0^{T-h} \|u(t+h) - u(t)\|_{W^{-1,1}}\, dt \mid u \in F\} = 0$.

To satisfy the first condition it suffices to show that the convex hull of $\{0\}$ and $\mathcal{S}$ is a compact subset of $W^{-1,1}(\Omega)$. But this is a direct consequence from Lemma B.3 since it is a compact set in $L^\infty(\Omega)$ endowed with the weak* topology.

For the second condition we can estimate

$$\begin{aligned} &\int_0^{T-h} \|u(t+h) - u(t)\|_{W^{-1,1}(\Omega)}\, dt \leq \int_0^t \|u(t+h) - u(t)\|_{L^1(\Omega)}\, dt \\ \leq\ &\int_0^h \int_0^{t-h} \|\dot{u}(t+s)\|_{L^1(\Omega)}\, dt\, ds \leq h \|u\|_{BV([0,T],L^1(\Omega))}. \end{aligned}$$

It remains to prove that the accumulation points are already contained in $\mathcal{T}$. First recall that $\mathcal{S}$ is a closed subset of $C_c^\infty(\Omega)'$. From $\lim_{n\to\infty} \int_0^T \|u_n(t) - u(t)\|_{W^{-1,1}(\Omega)}\, dt = 0$ follows that $\lim_{n\to\infty} u_n(t) = u(t)$ for a.e. $t \in [0,T]$, thus $u(t) \in \mathcal{S}$ almost everywhere. For an arbitrary test function $\varphi \in C_c^1([0,T], L^\infty(\Omega))$ we obtain

$$\int_0^T \int_\Omega u(t,x) \cdot \dot{\varphi}(t,x)\, dx\, dt = \lim_{n\to\infty} \int_0^T \int_\Omega u_n(t,x) \cdot \dot{\varphi}(t,x)\, dx\, dt \leq 1$$

since $\|u_n\|_{BV} \leq 1$ holds. This establishes our claim. QED

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