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A Variational Formulation of Rate-Independent Phase Transformations Using an Extremum Principle

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Dedicated to Erwin Stein on the occasion of his seventieth birthday

Abstract

We propose a rate-independent, mesoscopic model for the hysteretic evolution of phase transformations in shape-memory alloys. The model uses the deformation and phase-indicator function as basic unknowns and the potentials for the elastic energy and for the dissipation as constitutive laws. Using the associated functionals, admissible processes are defined to be the ones which are stable at all times and which satisfy the energy inequality.

This concept leads to a natural time-incremental method which consists in a minimization problem. The mesoscopic model is obtained by a relaxation procedure. It leads to new functionals involving the cross-quasiconvexification of the elastic stored-energy density. For a special case involving two phases of linearized elastic materials we show that the incremental problem provides existence of admissible processes for the time-continuous problem, if we let the time-step go to 0.

1. Introduction

In this paper we present a mathematical approach to the modeling of phase transformations (PT) in certain elastic materials, like martensitic PT in shape-memory alloys. In fact, the methodology introduced here applies to many other continuum mechanical models with inelastic behavior described by internal variables, like elasto-plasticity, damage, fracture or micromagnetism [FrM93, CHM02, FrM98, RoK02, Mi02a]. This paper contains three threads which run strongly intertwined through this work. First, we want to present a simple multi-dimensional model for the slow evolution of PT processes in solids which are able to describe hysteresis phenomena. Second, we discuss a general relaxation method for rate-independent time-evolution processes which are ill posed in their original form due to the formation of microstructure. Third, we show that the derived evolution problem can be analyzed in some special nontrivial cases, thus obtaining nontrivial existence results.

Elastic materials which allow for PT (like single or poly-crystalline shape-memory alloys) display hysteresis effects under quasistatic loading cycles. While there are many engineering models for this phenomenon for both uniaxial and multi-axial loading (see, e.g., [Wil93, HuM93, Lev94, LeS97, KMS99] and the references therein), mathematically rigorous models are only developed for simplified situations. On the one hand there is an extensive body of mathematical work on spatially one-dimensional situations (uniaxial case), see, e.g., [BrS96, MüS01, KuM00]. On the other hand there is a rich mathematical literature on static problems for the multi-dimensional situation. Most of that work is restricted to zero-stress or zero-energy solutions where the crystallographic properties and the transformation strain tensors determine the set of reachable macroscopic strains, see, e.g., [BaJ87, BaJ92, Bha93, BhK96, Mül99]. Models coming closer to our theory are given in [HaG99, Rou00, GoM01, Rou02].

So far there is no mathematical treatment of models which combine the hysteretic behavior with three-dimensional models of elasticity. Here we make a first proposal for combining these two features: (i) our model is truly three-dimensional, (ii) it has hysteretic behavior and (iii) it can deal with nonzero stresses. The model is derived from very simple mechanical postulates, namely a thermodynamic PT criterion and a definition of stable thermodynamic states. In the present version we neglect all thermal effects (isothermal case) and also all plastic effects. Of course, our model is crude and should be considered as the simplest nontrivial model rather than a realistic model for specific shape-memory alloys. It certainly will be a basis for more elaborate models.

The second theme of this paper is the relaxation of time-evolution processes which are mathematically ill posed. This ill-posedness is due to the formation of microstructure which usually arises from neglecting microscopical effects which would bound the smallest scales. On a mesoscopic scale we see formation of very small scales which have to be described in an averaged sense by relaxation. Here we treat rate-independent processes and approximate them by a fully implicit incremental problem (as is often used in engineering for plasticity problems) which for each step takes the form of a minimization problem. These problems can be relaxed introducing a phase-mixture theory. The resulting relaxed incremental problem can be understood as the incremental formulation of a time-continuous evolution problem for the phase mixtures.

This part is written in a very general and sometimes less rigorous way to see that it is a general program which opens up new ways to relax evolutionary problems derived from energy principles. Classical models in linearized elasto-plasticity can be formulated using this methodology, cf. [HaR95, ACZ99]. More recent work in [CHM02, Mi02a] applies these ideas to nonlinear elasto-plasticity (with finite strains).

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.

The third theme in the paper is devoted to a specific example, which allows for an existence theory. This is an example of solid–solid PT with two phases, where

each phase can be described by linearized elasticity and both phases have the same elasticity tensor but different transformation strains. For this case we show that most steps in the relaxation procedure can be made rigorous and we obtain an existence theorem for the relaxed time-continuous model. Here we use the general theory of rate-independent hysteresis which was developed in [MiT02] and is based on energetic formulations. This abstract theory is sketched in Section 2, since it is essential for the understanding of the relaxation procedure as well.

To be more specific, we describe the underlying mechanical model. 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 $P^{\mathrm{p}} = \{e_1, \dots, e_n\}$ is the set of all possible pure phases. The material 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 it is often assumed that $W_{e_j}(F) = W(FT_j^{-1})$ with a fixed energy density W, where T_j are the transformation strains for the martensitic phases (e.g., $n = 3$ for the cubic to tetragonal PT and $n = 12$ for the cubic to monoclinic PT, see [BhK96]). The matrices T_j are related to each other by the crystallographic symmetry group.

A function $c^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}$ is called an *internal state* of the system; however we will just call it a "state" subsequently. The superscript $^{\mathrm{p}}$ denotes *pure* and indicates the fact that at the present stage phase mixtures are not taken into account, i.e., at every point $x \in \Omega$ the material is in a pure phase. For the loading $G(t)$ and a deformation $u : \Omega \to \mathbb{R}^d$ the elastic plus potential energy defines the energy functional (Gibbs energy)

$$\mathcal{E}^{\mathrm{p}}(t, c^{\mathrm{p}}, u) = \int_\Omega W_{c^{\mathrm{p}}(x)}(\nabla u(x))\,\mathrm{d}x - \langle G(t), u\rangle$$

with $\langle G(t), u\rangle = \int_\Omega f_{\mathrm{vol}}(t, x) \cdot u(x)\,\mathrm{d}x + \int_{\partial\Omega\setminus\Gamma} g_{\mathrm{surf}}(t, y) \cdot u(y)\,\mathrm{d}a(y)$. We denote by $\mathcal{V} = \left\{ u \in \mathrm{W}^{1,p}(\Omega) \mid u|_\Gamma = u_{\mathrm{Dir}} \right\}$ the set of kinematically admissible deformations. A basic assumption for rate-independent processes is that for all time the elastic deformation is stable. Hence, we define the reduced energy functional

$$\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}) = \inf \left\{ \mathcal{E}^{\mathrm{p}}(t, c^{\mathrm{p}}, u) \mid u \in \mathcal{V} \right\},$$

which assumes that $u(t)$ is always a global minimizer of $\mathcal{E}^{\mathrm{p}}(t, c^{\mathrm{p}}, \cdot)$. Hence, $\mathcal{I}^{\mathrm{p}}$ describes the elastic properties of the body in terms of the state c^{p}.

Next we model the dissipation due to changes in the state c^{p}. We postulate the existence of dissipation coefficients $\kappa_{i\to j}$ measuring the dissipation per unit volume for a PT from e_i into e_j and satisfying $\kappa_{j\to j} = 0$, and $\kappa_{i\to j} > 0$ for $j \neq i$. Under the assumption that at most one PT occurs at each material point the bulk dissipation of a PT from state $a^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}$ into $c^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}$ is

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

A family of states $(c^{\mathrm{p}}(t))_{t\in[0,T]}$ is called a process, and the total amount of dissipation due to PT in the time interval $[t_1, t_2]$ is denoted by $\mathrm{Diss}^{\mathrm{p}}(c^{\mathrm{p}}; t_1, t_2)$.

One mechanical motivation of such a rate-independent dissipation is athermal resistance against interface motion as described in [GhO94]. Athermal resistance

is similar to dry friction, i.e., PT from e_i to e_j can start when the driving force exceeds the dissipative threshold $\kappa_{i\to j}$, independently of the interface velocity. It is caused by the interaction of interfaces with obstacles having long-range stress fields (point defects, dislocations, grains, twins and subgrain boundaries) which cannot be overcome by thermal fluctuations. Short-range resistance which can be overcome by thermal activation gives rise to rate-dependent or viscous friction, which is not taken into account here. A phenomenological motivation for this type of dry friction arises from the modeling of systems with potential wells. If a system stays in local (but not global) minima as long as possible then the energy difference between the saddle point separating the two wells and the new minimum will be dissipated in this PT, see Section 3.1.

Having the two constitutive functionals $\mathcal{I}^{\mathrm{p}}$ and $\mathcal{D}^{\mathrm{p}}$, we then have to find an evolution law for the process $c^{\mathrm{p}}(t)$. Here we use an *extremum principle* to determine which PT out of the set of all possible PT does occur, that is, what phases are created in what regions. This principle was formulated in [Lev95, Lev97, Lev98, Lev00] in a more general context also allowing for plastic effects and is called the *postulate of realizability*. Restricted to our case, it says that PT occurs as soon as it is thermodynamically possible, namely when the gain in energy through a PT from a state a^{p} to b^{p} is larger than (or equal to) the dissipated energy: $\mathcal{I}^{\mathrm{p}}(t, a^{\mathrm{p}}) - \mathcal{I}^{\mathrm{p}}(t, b^{\mathrm{p}}) > \mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, b^{\mathrm{p}})$. Here, the main assumption is that there are no other sources of dissipation.

Hence, an observable process $(c^{\mathrm{p}}(t))_{t\in[0,T]}$ must be *stable* for all $t \in [0, T]$, i.e.,

$$\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}(t)) \leqq \mathcal{I}^{\mathrm{p}}(t, b^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}(t), b^{\mathrm{p}}) \quad \text{for all } b^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}.$$

It is surprising that this condition together with the *energy inequality*

$$\mathcal{I}^{\mathrm{p}}(t_2, c^{\mathrm{p}}(t_2)) + \mathrm{Diss}^{\mathrm{p}}(c^{\mathrm{p}}; t_1, t_2) \leqq \mathcal{I}^{\mathrm{p}}(t_1, c^{\mathrm{p}}(t_1)) - \int_{t_1}^{t_2} \langle \dot{G}(s), u(s)\rangle \,\mathrm{d}s$$

suffices to characterize the evolution of the problem. We are lead to the following time-continuous formulation of the extremum principle.

(CP) For given c_0^{p}, find a process $c^{\mathrm{p}} : [0, T] \times \Omega \to P^{\mathrm{p}}$ with $c^{\mathrm{p}}(0, x) = c_0^{\mathrm{p}}(x)$ which is stable and satisfies the energy inequality for all $0 \leqq t_1 < t_2 \leqq T$.

At this point we want to connect our theory to the purely static theory of PT without dissipation which is an active mathematical subject, see [BaJ87, BaJ92] and the survey [Mül99]. For our mechanical situation it would mean considering the single stored-energy density

$$\overline{W}(F) = \min\left\{ W_{e_j}(F) \mid j = 1, \dots, n \right\},$$

which is not quasiconvex but has potential wells in the sets $\mathrm{SO}(3)T_j$. In general, the infimum of the functional $\overline{\mathcal{E}}(t, u) = \int_\Omega \overline{W}(\nabla u(x))\,\mathrm{d}x - \langle G(t), u\rangle$ is not attained since infimizing sequences develop finer and finer oscillations in the function c^{p} defined via $\overline{W}(\nabla u(x)) = W_{c^{\mathrm{p}}(x)}(\nabla u(x))$. This problem can be avoided by considering a suitable relaxation $R\overline{\mathcal{E}}(t, \cdot)$, namely the lower semicontinuous envelope,

[Dac89]. However, if we always look for global minimizers we cannot obtain hysteretic behavior in rate-independent loading processes as no time direction is preferred. Nevertheless hysteretic behavior occurs (see [BCJ95]) due to local strong minimizers which have a true potential barrier in a suitable function space. To describe this phenomenon with our approach we have to keep track of the internal variable c^{p} and to choose a dissipation functional $\mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}})$ such that for each such local strong minimizer u the associated phase function $c_u^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}$ is a global minimum of $a^{\mathrm{p}} \mapsto \mathcal{I}^{\mathrm{p}}(t, a^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_u^{\mathrm{p}}, a^{\mathrm{p}})$. In Section 3.1 we discuss the relation between models with internal variables c^{p} and models without but having potential barriers.

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 $c^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}$. A natural way to find stable states at time t is to minimize $\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}})$ over all c^{p}. Clearly such a minimizer must be stable; however, in general we can only expect to find an infimizing sequence c_j^{p}, i.e., $\mathcal{I}^{\mathrm{p}}(t, c_j^{\mathrm{p}}) \to \alpha = \inf\{\mathcal{I}^{\mathrm{p}}(t, b^{\mathrm{p}}) \mid b^{\mathrm{p}} : \Omega \to P^{\mathrm{p}}\}$. The weak limit c of the sequence c_j^{p} 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^{p} with $c^{\mathrm{p}}(t, x) \in P^{\mathrm{p}}$ to phase mixtures c with $c(t, x) \in P$ where

$$P = \mathrm{conv}(P^{\mathrm{p}}) = \left\{ c \in \mathbb{R}^n \;\middle|\; c = \sum_{j=1}^{n} \theta_j e_j,\ \theta_j \geqq 0,\ \sum_{j=1}^{n} \theta_j = 1 \right\}.$$

In mathematical terms such a procedure is called relaxation. We emphasize 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.

The main idea for finding a 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. Relaxation of a single variational problem is a well-developed theory, cf. [Dac89, Rou97]; however for incremental problems no suitable generalization is known. The problem is to control the interaction of the microstructures on different time levels, see [FrM93, FrM98] for a first discussion in the context of fracture. In Section 4.1.2 we propose an abstract setting for relaxations of incremental problems, for general evolution problems a counterpart is discussed in [The01, Mi02b]. However, to obtain a tractable model we propose a separately relaxed incremental problem (SRIP) which, in general, does not coincide with the mathematical relaxation, but see [The01] for a rigorous justifications in special cases. In our setting, separate relaxation tends to neglect incompatibilities between the microstructures of the phase mixtures at two subsequent time-steps, and therefore underestimate the true dissipation (making hysteretic effects smaller). For more general philosophy of relaxation of rate-independent problems we refer to [The01, Mi02b].

The major advantage of (SRIP) is that it is explicit enough to give an efficient solution algorithm and to prove existence results. Moreover, its form immediately shows that it is the time discretization of a time-continuous relaxed problem (SRCP).

To describe the separately relaxed problem we start with the unrelaxed *incremental problem* (IP) for a given partition $0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T$:

(IP) For given c_0^{p}, find c_k^{p} such that $\mathcal{I}^{\mathrm{p}}(t_k, c_k^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_{k-1}^{\mathrm{p}}, c_k^{\mathrm{p}})$ is minimal for $k = 1, \dots, N$.

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 the same reason as mentioned above for (CP). Here (CP) and (IP) are defined on the set $\mathcal{P}^{\mathrm{p}} = \mathrm{L}^1(\Omega, P^{\mathrm{p}})$ of pure states, whose weak closure is the convex set $\mathcal{P} = \mathrm{L}^1(\Omega, P)$ of mixture states. The separate relaxed incremental problem is now obtained by relaxing the functionals $\mathcal{I}^{\mathrm{p}}(t, \cdot) : \mathcal{P}^{\mathrm{p}} \to \mathbb{R}$ and $\mathcal{D}^{\mathrm{p}} : \mathcal{P}^{\mathrm{p}} \times \mathcal{P}^{\mathrm{p}} \to \mathbb{R}$ independently leading to the relaxations $\mathcal{I}(t, \cdot) : \mathcal{P} \to \mathbb{R}$ and $\mathcal{D} : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$. Now, the *separately relaxed incremental problem* is formulated in $\mathcal{P} = \mathrm{L}^1(\Omega, P)$ and reads

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

By construction $\mathcal{I}$ and $\mathcal{D}$ are lower semicontinuous, which implies that (SRIP) is always solvable.

An important fact is that $\mathcal{I}$ and $\mathcal{D}$ can be characterized nicely. We have

$$\mathcal{I}(t, c) = \inf \left\{ \int_\Omega \mathbb{W}(c(x), \nabla u(x))\,\mathrm{d}x - \langle G(t), u\rangle \;\middle|\; u \in \mathcal{V} \right\},$$

where the *mixture function* is defined, using solely W_{e_i}, $i = 1, \dots, n$, via

$$\mathbb{W}(c, F) = \inf \left\{ \fint_B W_{c^{\mathrm{p}}(y)}(F + \nabla\phi(y))\mathrm{d}y \;\middle|\; \fint_B c^{\mathrm{p}}(y)\mathrm{d}y = c, \right.$$
$$\left. c^{\mathrm{p}} \in \mathrm{L}^1(\Omega, P^{\mathrm{p}}),\ \phi \in \mathrm{W}_0^{1,p}(B) \right\}.$$

For given $c \in P$ this function describes the elastic properties of optimally arranged mixtures with macroscopic phase portions c. This mixture function is not postulated but follows from an exact mathematical theory which is similar to homogenization theory, cf. [Koh91, FKP94, SmW98, Mie00]. In [LeR00], $\mathbb{W}$ is called *cross-quasiconvexification*; see Section 4.2 for more details.

The relaxed dissipation functional takes the form

$$\mathcal{D}(a, c) = \mathbf{\Delta}(c - a) \quad \text{with} \quad \mathbf{\Delta}(z) = \int_\Omega \Delta(z(x))\,\mathrm{d}x, \tag{1.1}$$

where $\Delta : \mathbb{R}^n \to \mathbb{R}_{\geqq}$ is piecewise affine, convex, homogeneous of degree 1 and satisfies $\Delta(e_j - e_i) = D(e_i, e_j) = \kappa_{i\to j}$; see Section 4.3 for more details.

The minimization in (SRIP) is a simultaneous minimization on c and u which has the advantage that c appears only locally under the integral. Hence, the minimization with respect to c can be done pointwise first and then u can be determined. This leads to the numerically useful algorithm (SRIP)′, see Section 4.4 and [MTL98, CaP00].

The structure of (SRIP) shows that it is nothing else than the incremental version of the following time-continuous problem (SRCP). In analogy to the pure phase situation we say that $c : [0, T] \to \mathrm{L}^1(\Omega, P)$ is stable, if

$$\mathcal{I}(t, c(t)) \leqq \mathcal{I}(t, a) + \mathbf{\Delta}(a - c(t)) \quad \text{for } t \in [0, T] \text{ and } a \in \mathrm{L}^1(\Omega, P). \tag{1.2}$$

Since $\mathbf{\Delta}$ is defined on the Banach space $\mathrm{L}^1(\Omega, P)$, the dissipation of a process takes the form $\int_{t_1}^{t_2} \mathbf{\Delta}(\mathrm{d}c) = \sup \sum_{k=1}^{N} \mathbf{\Delta}(c(t_k) - c(t_{k-1}))$ where the supremum is taken over all partitions. The energy inequality for c now takes the form

$$\mathcal{I}(t_2, c(t_2)) + \int_{t_1}^{t_2} \mathbf{\Delta}(\mathrm{d}c) \leqq \mathcal{I}(t_1, c(t_1)) + \int_{t_1}^{t_2} \partial_t \mathcal{I}(s, c(s))\, \mathrm{d}s. \tag{1.3}$$

With these definitions the *separately relaxed time-continuous problem* reads:

(SRCP) For given c_0, find $c : [0, T] \to \mathcal{P}$ with $c(0) = c_0$ such that stability (1.2) and energy inequality (1.3) holds for $0 \leqq t_1 < t_2 \leqq T$.

In Section 5 we study a special PT example given by two phases which are both modeled by linearized elasticity with the same elastic tensor. For this example, with a few more specifications, we are able to show that (SRCP) has a solution for all initial data $c_0 \in \mathcal{P}$. Here we use the fact that $\mathbb{W}$ is explicitly known and is quadratic in ∇u and $\theta \in [0, 1]$ where $c = (1-\theta, \theta)^T$ ($\mathcal{P}$ can be identified with $\mathrm{L}^1(\Omega, [0, 1])$). Thus, $\mathcal{I}(t, \cdot) : \mathcal{P} \to \mathbb{R}$ is quadratic as well; yet the problem remains strongly nonlinear due to the constraint $c \in \mathcal{P}$.

The existence proof is based on the abstract methods for rate-independent problems which are worked out in Section 2 and given in more detail in [MiT02]. The basic idea is to solve the incremental problem (SRIP) for finer and finer time discretizations giving piecewise-constant approximations c^N. Using the energy inequality, which also holds for (SRIP), we find the *a priori* bound

$$\int_0^T \mathbf{\Delta}(\mathrm{d}c^N) = \sum_{k=1}^{N} \mathbf{\Delta}(c(t_k^N) - c(t_{k-1}^N)) \leqq C^*,$$

where C^* is independent of N. Because of $\|z\|_{\mathrm{L}^1(\Omega)} \leqq C\mathbf{\Delta}(z)$ the sequence c^N is bounded in $\mathrm{BV}([0, T], L^1(\Omega))$, and an adaption of Helly's selection principle provides a subsequence c^{N_l} and a limit c^∞ such that $c^{N_l}(t) \rightharpoonup c^\infty(t)$ in $L^1(\Omega)$. (Note that rate independence and (1.1) forces us to use the L^1 setting, although the weak and the strong topology on $\mathrm{L}^1(\Omega, P)$ coincide with those on $\mathrm{L}^q(\Omega, P)$ for all $q \in (1, \infty)$.) It is easy to see that c^∞ satisfies the energy inequality (1.3) for $t_1 = 0$ and $t_2 = T$. However, to show that c^∞ is also stable requires a further compactness argument in the spatial direction. This is derived using pseudo-differential operators and H-measures, cf. [Tar90, Ger91].

Having established a mathematical model which enables us to study simultaneously hysteretic and multi-dimensional effects, it is possible to study the question of their interaction. In [KMS99, CaP00, GoM01, GMH02] numerical implementations of the models developed here are discussed, tested and compared with experiments. In particular it is important to investigate whether multi-dimensional models display

a richer class of hysteresis effects and whether it is really necessary to introduce more internal variables to explain the more complicated hysteresis loops observed in uniaxial experiments, cf. [Wil93, Lev94, MüS01, KuM00].

2. Rate-independent processes

The mathematical framework is based on two abstract energy functionals

$$\mathcal{I} : [0, T] \times X \to \mathbb{R} \qquad \text{and} \qquad \mathbf{\Delta} : X \to \mathbb{R}_{\geqq} = [0, \infty),$$

which represent the potential energy of a state $c \in X$ and the dissipation power caused by a rate $\dot{c} \in X$, both lying in the Banach space X. The dissipation potential $\mathbf{\Delta}$ is convex and homogenous of degree 1, which leads to rate independence. For differentiable functionals $\mathcal{I}$ there exists a rich amount of literature devoted to differential inclusions of the form

$$-\mathrm{D}\mathcal{I}(t, c) \in \partial \mathbf{\Delta}(\dot{c}), \tag{2.1}$$

see, e.g., [BrS96, Vis94] for a starting point. Here ∂ denotes the subdifferential operator for convex functions, cf. Definition 2.2. The evolution equation (2.1) is a very general model for systems with hysteresis (like elasto-plastic or magnetic materials). For time-independent functionals $\mathcal{I}$ the Cauchy problem is trivial, every constant process $c(t) \equiv c_0$, where c_0 satisfies $-\mathrm{D}\mathcal{I}(c_0) \in \partial \mathbf{\Delta}(0)$, is a solution. The time dependence of $\mathcal{I}$ describes the change of the external loading. For time-dependent functionals $\mathcal{I}$ system (2.1) constitutes the limit equation for the response to very small loading rates when inertial effects and relaxation effects disappear, i.e., the system response is immediate. Only the stick-slip motion due to the dry friction is left. Formally the system is able to take into account all the spatial effects which affect the hysteretic behavior but unfortunately global well-posedness can only be expected in special cases. One of the most prominent mathematical difficulties is that solutions might be discontinuous in time if the potential energy $\mathcal{I}$ is not strictly convex. The case where $\mathcal{I}$ is uniformly convex and smooth is well understood and leads to well-posedness of the Cauchy problem, see [MiT02]. In this section we will derive a new sufficient condition for existence of solutions to a reformulated version of (2.1) where also the case $\mathcal{I} : [0, T] \times X \to \mathbb{R} \cup \{\infty\}$ can be treated. Our new condition is independent of convexity of $\mathcal{I}$, therefore we hope to be able to handle situations in continuum mechanics where convexity contradicts the fundamental principle of invariance under rigid body rotations. Uniqueness of solutions lies outside of the scope of this work. In Chapter 5, for a special example which models the dynamics of martensitic PT in solids, we will demonstrate that our new condition actually holds and consequently the existence of solutions can be established.

2.1. Setup of the problem

Let X be a separable Banach space with dual space X^* and let $\mathcal{P}$ be a weakly closed subset of X. For every time $t \in [0, T]$ where T is a fixed positive number and

every $c \in \mathcal{P}$ the energy of the state c is given by the *energy functional* $\mathcal{I}(t, c) \in \mathbb{R}_{\geqq}$. For $\mathcal{I}$ we assume the following properties:

$$\mathcal{I} \in \mathrm{C}^0([0, T] \times \mathcal{P}), \qquad \sup_{c \in \mathcal{P}, t \in [0,T]} |\partial_t \mathcal{I}(t, c)| < \infty, \tag{2.2}$$

$$\text{for every } t \in [0, T] \text{ the mapping } c \mapsto \mathcal{I}(t, c) \text{ is weakly lower semicontinuous.} \tag{2.3}$$

In the PT problem the restriction of the phase space to $\mathcal{P} \subset X$ accounts for the fact that the variable c measures the concentration of phases, i.e., $c(t, x) \in P \subset \mathbb{R}^n$. This restriction is far more than a technical modification of the usual setting, e.g., in the theory of linearized elasto-plasticity where $\mathcal{P} = X$. If $\mathcal{P}$ is bounded, the set of tangential directions may become abruptly smaller as the state c reaches the boundary of $\mathcal{P}$. As a positive effect, the set $\mathcal{P}$ may be weakly compact although X is not reflexive, and this simplifies central steps of the analysis.

Most of our work will take place in spaces of bounded variation in time,

$$\mathrm{BV}([0, T], \mathcal{P}) = \{\, f : [0, T] \to \mathcal{P} \mid \mathrm{Var}(f; [0, T]) < \infty \,\}$$

with $\mathrm{Var}(f; [0, T]) = \sup \sum_{k=0}^{N-1} \|f(t_{k+1}) - f(t_k)\|$ where the supremum is taken over all $N \in \mathbb{N}$ and all partitions with $0 = t_0 < \ldots < t_N = T$. Observe that our definition of BV functions does not neglect sets of measure 0, therefore $\mathrm{BV}([0, T], X)$ is larger than $\mathrm{C}^0([0, T], X^*)^*$, even if X is reflexive or finite dimensional.

The dissipation generated by c changing from one state to a different state is given by a *dissipation functional* $\mathbf{\Delta} : X \to \mathbb{R}_{\geqq}$ which is convex and homogeneous of degree 1. In the literature (see, e.g., [GNS83]) $\mathbf{\Delta}$ is also denoted as *pseudo-potential*, since it takes a rate as an argument. We assume that there exists $C > 0$ so that

$$\|v\|/C \leqq \mathbf{\Delta}(v) \leqq C\|v\|. \tag{2.4}$$

It will become clear later that in our model the solutions are rate independent if and only if the $\mathbf{\Delta}$ is homogeneous of degree one. An immediate consequence of the convexity and the homogeneity of $\mathbf{\Delta}$ is the triangle inequality

$$\mathbf{\Delta}(v_1 + v_2) \leqq \mathbf{\Delta}(v_1) + \mathbf{\Delta}(v_2) \quad \text{for every } v_1, v_2 \in X. \tag{2.5}$$

In continuum mechanics $\mathbf{\Delta}$ is obtained by integration over Ω, i.e., $\mathbf{\Delta}(v) = \int_\Omega \Delta(v(x))\, \mathrm{d}x$; hence, (2.4) can only hold if X equals $\mathrm{L}^1(\Omega, \mathbb{R}^n)$. A state c is called *stable* at time t if

$$\mathcal{I}(t, c) \leqq \mathcal{I}(t, a) + \mathbf{\Delta}(a - c) \quad \text{for every } a \in \mathcal{P}. \tag{S}$$

The variation of a BV function f with respect to the functional $\mathbf{\Delta}$ is written as

$$\int_0^T \mathbf{\Delta}(\mathrm{d}f) \stackrel{\text{def}}{=} \sup_{0 = t_0 < \ldots < t_N = T} \sum_{k=0}^{N-1} \mathbf{\Delta}(f(t_{k+1}) - f(t_k)).$$

By (2.4) we have $\mathrm{Var}(f;[0,T])/C \leqq \int_0^T \mathbf{\Delta}(\mathrm{d}f) \leqq C\mathrm{Var}(f,[0,T])$. A process $c \in \mathrm{BV}([0,T],\mathcal{P})$ satisfies the *energy inequality* if, for all t_1, t_2 with $0 \leqq t_1 < t_2 \leqq T$, we have

$$\mathcal{I}(t_2,c(t_2)) + \int_{t_1}^{t_2} \mathbf{\Delta}(\mathrm{d}c) \leqq \mathcal{I}(t_1,c(t_1)) + \int_{t_1}^{t_2} \partial_t \mathcal{I}(t,c(t))\,\mathrm{d}t \tag{E}$$

holds. We say that c satisfies the *weak energy inequality* if (E) holds just for $t_1 = 0$ and $t_2 = T$.

This energetic formulation requires no differentiability for $\mathcal{I}(t,\cdot)$ and $c(\cdot)$. The central problem in this work is the construction of processes which satisfy both (S) and (E).

Definition 2.1. For every $t \in [0,T]$ we denote by $\mathcal{S}(t) \subset \mathcal{P}$ the *set of stable points*,

$$\mathcal{S}(t) \stackrel{\mathrm{def}}{=} \left\{ c \in \mathcal{P} \mid \mathcal{I}(t,c) \leqq \mathcal{I}(t,a) + \mathbf{\Delta}(a-c)\ \forall a \in \mathcal{P} \right\}.$$

A process $c \in \mathrm{BV}([0,T],\mathcal{P})$ is called *stable* if $c(t) \in \mathcal{S}(t)$ for every $t \in (0,T]$. Stable processes which satisfy (E) are called *admissible* for $\mathcal{I}$ and $\mathbf{\Delta}$.

The definition of admissibility satisfies the two standard properties of the term "solution" in evolutionary systems, when no uniqueness of the Cauchy problem is assumed.

1. *Restriction property.* For every admissible $c : [0,T] \to \mathcal{P}$ and every $[s,t] \subset [0,T]$ the restriction $c|_{[s,t]}$ is admissible as well.
2. *Concatenation property.* Assume that $c_1 : [t_1,t_2] \to \mathcal{P}$ and $c_2 : [t_2,t_3] \to \mathcal{P}$ are admissible and that $c_1(t_2) = c_2(t_2)$. Then the concatenation $\widetilde{c} : [t_1,t_3] \to \mathcal{P}$ is admissible as well, where $\widetilde{c}(t) = c_1(t)$ if $t \in [t_1,t_2]$ and $\widetilde{c}(t) = c_2(t)$ if $t \in [t_2,t_3]$.

In the case of convex potential energies $\mathcal{I}(t,\cdot)$ the above energetic definition of admissibility is equivalent to certain local formulations using variational inequalities or differential inclusions.

Definition 2.2. For a convex function $\mathcal{J} : X \to \mathbb{R} \cup \{\infty\}$ the *subdifferential* at c is the set

$$\partial\mathcal{J}(c) = \left\{ \sigma \in X^* \mid \mathcal{J}(a) \geqq \mathcal{J}(c) + \langle \sigma, a-c \rangle \text{ for all } a \in X \right\}.$$

The *indicator function* $\mathcal{X}_A$ of a set $A \subset X$ is defined by $\mathcal{X}_A(a) = 0$ for $a \in A$ and $\mathcal{X}_A(x) = \infty$ for $x \in X \setminus A$. For a convex set $\mathcal{P} \subset X$ the (interior) *tangent cone* $\mathrm{T}_c\mathcal{P}$ of $\mathcal{P}$ at $c \in \mathcal{P}$ is given by

$$\mathrm{T}_c\mathcal{P} = \mathrm{closure}_X\Big(\{ v \in X \mid \exists \lambda > 0 :\ c + \lambda v \in \mathcal{P} \} \Big),$$

and the (outer) *normal cone* is given by

$$\mathrm{N}_c\mathcal{P} = \left\{ \sigma \in X^* \mid \langle \sigma, v \rangle \leqq 0 \text{ for all } v \in \mathrm{T}_c\mathcal{P} \right\}.$$

It is well known that for closed convex sets $\mathcal{P} \subset X$ we have $\partial \mathcal{X}_{\mathcal{P}}(c) = \mathrm{N}_c\mathcal{P}$.

For simplicity we have restricted the following result to processes $c : [0, T] \to \mathcal{P}$ which are absolutely continuous. For the case of general $c \in \mathrm{BV}([0, T], X)$ there is a corresponding result if (renormalized) directional derivatives are used and the jumps are handled properly. We refer to [MiT02], where also the complete proof can be found.

Theorem 2.3 (Equivalence between the energetic and local formulations**).** *Let X be a Banach space and $\mathcal{P} \subset X$ convex and weakly closed. Let the functional $\mathcal{I} \in C^1([0, T]\times\mathcal{P})$ be convex and satisfy* (2.2). *Let the functional $\mathbf{\Delta} : X \to \mathbb{R}$ be convex and coercive in the sense of* (2.4). *Then for $c \in \mathrm{W}^{1,1}((0, T), X) \cap \mathrm{C}([0, T], \mathcal{P})$ the following statements are equivalent:*

(i) *c satisfies* (S) *and* (E)*;*
(ii) *c satisfies for almost all $t \in [0, T]$ the local version of* (S) *and* (E)*, namely*

$$\langle \mathrm{D}\mathcal{I}(t, c(t)), v\rangle + \mathbf{\Delta}(v) \geqq 0 \quad \textit{for all } v \in \mathrm{T}_{c(t)}\mathcal{P}, \tag{2.6}$$

$$\langle \mathrm{D}\mathcal{I}(t, c(t)), \dot{c}\rangle + \mathbf{\Delta}(\dot{c}) \leqq 0; \tag{2.7}$$

(iii) *c is a solution for the differential inclusion*

$$0 \in \partial\mathbf{\Delta}(\dot{c}(t)) + \mathrm{D}\mathcal{I}(t, c(t)) + \partial\mathcal{X}_{\mathcal{P}}(c(t)) \quad \textit{for almost all } t \in [0, T]. \tag{2.8}$$

In the case of general convex $\mathcal{I}(t, \cdot)$, which need not be differentiable, the subdifferential allows for a formulation of the problem as a differential inclusion:

$$0 \in \partial\mathbf{\Delta}(\dot{c}(t)) + \partial(\mathcal{I}(t, \cdot)+\mathcal{X}_{\mathcal{P}})(c(t)) \text{ for a.e. } t \in [0, T]. \tag{2.9}$$

With the relation $\partial(\mathcal{I}(t, \cdot)+\mathcal{X}_{\mathcal{P}}) = \partial\mathcal{I}(t, \cdot) + \partial\mathcal{X}_{\mathcal{P}} = \partial\mathcal{I}(t, \cdot) + \mathrm{N}\mathcal{P}$ this means

$$\exists\, \widetilde{\sigma}(t) \in \partial\mathcal{I}(t, c(t))\ \exists\, \widetilde{n}(t) \in \mathrm{N}_{c(t)}\mathcal{P} :\ -\widetilde{\sigma}(t) - \widetilde{n}(t) \in \partial\mathbf{\Delta}(\dot{c}(t)).$$

Here $-\widetilde{\sigma}(t)$ can be understood as the conjugate force to the variable c, and $-\widetilde{n}(t)$ is the reaction of the boundary of $\mathcal{P}$. Clearly the sum of both has to be equal to the dissipative force. We will use this formulation in Section 4.5 to derive a flow formulation for the phase-transformation problem, which is used in the engineering literature and which has a lot of similarities with flow rules in plasticity theory. However, since these flow formulations are not needed in what follows, we omit the details and refer to [MiT02, Mi02a].

When taking limits with respect to time we have to be careful about temporal discontinuities. By general theorems on BV functions we know that a BV function c has at most a countable number of discontinuities and that for each $t \in [0, T]$ the limit from the right and from the left exists. For c we define its projection c^- into the space of left-continuous BV functions via $c^-(0) = c(0)$ and $c^-(t) = \lim_{s\nearrow t} c(s)$ for $t \in (0, T]$ and find $\|c^-\|_{\mathrm{BV}([0,T],X)} \leqq \|c\|_{\mathrm{BV}([0,T],X)}$.

Lemma 2.4. *Under the assumptions* (2.2) *and* (2.4) *the stable set $\mathcal{S}(t)$ is a closed subset of $\mathcal{P}$ for all $t \in [0, T]$. Moreover, $\cup_{t\in[0,T]}(t, \mathcal{S}(t))$ is a closed subset of $[0, T] \times \mathcal{P}$. If a process $c \in \mathrm{BV}([0, T], \mathcal{P})$ is stable for all $t \in \mathcal{T}$, where $\mathcal{T}$ is a dense subset of $[0, T]$, then c^- is a stable process.*

Proof. We prove the second statement since the first is a consequence of the second. Assume $c^k \in \mathcal{S}(t_k)$ with $c^k \to c^*$ and $t_k \to t_*$. By the continuity of $\mathcal{I}$ and $\mathbf{\Delta}$ we have, for arbitrary $a \in \mathcal{P}$,

$$\begin{aligned}\mathcal{I}(t_*, c^*) &= \lim_{k\to\infty} \mathcal{I}(t_k, c^k) \leqq \liminf_{k\to\infty} (\mathcal{I}(t_k, a) + \mathbf{\Delta}(a - c^k)) \\ &= \mathcal{I}(t_*, a) + \mathbf{\Delta}(a - c_*).\end{aligned}$$

To prove the third statement let $t \in (0, T]$ and choose a sequence $(t_k)_{k\in\mathbb{N}}$ with $t_k \in \mathcal{T}$ and $t_k \nearrow t$. Then, $c^-(t) = \lim_{k\to\infty} c(t_k)$ and the result follows from the second statement. □

The next three subsections give an overview of the properties of admissible processes; for more details we refer to [MiT02].

2.2. Qualitative properties of admissible processes

At the jumps a process can take rather arbitrary values without violating (S) or (E). To obtain definiteness we restrict ourselves to functions which are continuous from the left, i.e., $c = c^-$. Assumption (2.4) gives a bound on the variation of c. Therefore the space $\mathrm{BV}([0, T], \mathcal{P})$ is the natural space to work within. From stability (S) and the weak energy inequality (E) we can infer that an energy identity holds on every subinterval.

Theorem 2.5. *Assume that the dissipation functional* $\mathbf{\Delta}$ *satisfies the coercivity assumption* (2.4) *for some positive constant* C *and that* (2.2) *holds. If* c *is a stable process with* $c = c^-$ *and satisfying the weak energy inequality* (E) (*i.e., only for* $t_1 = 0$ *and* $t_2 = T$), *then the energy equality*

$$\mathcal{I}(t, c(t)) + \int_s^t \mathbf{\Delta}(\mathrm{d}c) = \mathcal{I}(s, c(s)) + \int_s^t \partial_t \mathcal{I}(\tau, c(\tau))\,\mathrm{d}\tau \tag{2.10}$$

holds for every $0 \leqq s < t \leqq T$.

Proof. We set for $t_1, t_2 \in [0, T]$ the function $\mathcal{J}(t_1, t_2) = \mathcal{I}(t_1, c(t_2))$. Now for every $0 \leqq s \leqq t \leqq T$ we have

$$\begin{aligned}&\mathcal{I}(s, c(s)) - \mathcal{I}(t, c(t)) + \int_s^t \{\partial_t \mathcal{I}(\tau, c(\tau)) - \mathbf{\Delta}(\dot{c}(\tau))\}\,\mathrm{d}\tau \\ &\qquad = -\int_s^t \{\partial_{t_2} \mathcal{J}(\tau, \tau) + \mathbf{\Delta}(\dot{c}(\tau))\}\,\mathrm{d}\tau.\end{aligned}$$

By the last assumption the left-hand side is nonnegative if we let $s = 0$ and $t = T$. Therefore the claim follows if we can show that the integrand on the right-hand side is nonnegative in $C([0, T])^*$. The stability inequality (S) implies, for every $t \in [0, T)$ and $h \in (0, T - t)$,

$$\tfrac{1}{h}[\mathcal{I}(t, c(t+h)) - \mathcal{I}(t, c(t))] + \mathbf{\Delta}(\tfrac{1}{h}[c(t+h) - c(t)]) \geqq 0,$$

and this expression converges weak* to $t \mapsto \partial_{t_2} \mathcal{J}(t, t) + \mathbf{\Delta}(\dot{c}(t))$ as $h \to 0$. Since the set of positive functionals is weak* closed, the proof is finished. □

2.3. Existence of admissible processes

So far we have only discussed the qualitative properties of admissible processes without knowing whether they exist. The typical way to achieve existence is to discretize (S) and (E) fully implicitly in time. This gives a variational problem and in certain cases it is possible to show that that solutions to the discretized problem converge to an admissible process as the fineness of the time discretization tends to 0. It is surprising that the discretized problems seem to have more structure than the original system (E), (S) although no assumption on the differentiability of the potential $\mathcal{I}$ and the dissipation functional $\mathbf{\Delta}$ is made. Major parts of the work in the following sections are inspired by the time-discretized problem. Replacing $\dot{c}$, $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(t, c(t))$ and $\frac{\partial}{\partial t}\mathcal{I}(t, c)$ by the appropriate finite differences, we arrive immediately at the incremental problem

(IP) Given $c_0 \in \mathcal{P}$ and a time discretization $0 = t_0 < \ldots < t_N = T$, find for $k = 1 \ldots N$ states $c_k^N \in \mathcal{P}$ such that $\mathcal{I}(t_k, c_k^N) + \mathbf{\Delta}(c_k^N - c_{k-1}^N)$ is minimal.

To guarantee the existence of solutions to (IP) we need some compactness:

$$\text{For all } r > 0 \text{ the intersection } \mathcal{P} \cap \left\{ c \in X \mid \|c\| \leqq r \right\} \text{ is weakly compact in } X. \tag{2.11}$$

Defining $c^N : [0, T] \to \mathcal{P}$ as the left-continuous piecewise-constant interpolant satisfying $c^N(t) = c_k^N$ for $t \in (t_{k-1}, t_k]$ and $c^N(0) = c_0$, we obtain the following existence result.

Theorem 2.6. *If the assumptions* (2.2)–(2.4) *and* (2.11) *hold, then* (IP) *has a solution and for every solution to* (IP) *the following statements hold true:*

(i) *for every* $t \in \{t_1, \ldots, t_N = T\}$ *the state* $c^N(t)$ *is stable,*
(ii) c^N *satisfies the discrete energy inequality*

$$\mathcal{I}(T, c^N(T)) + \int_0^T \mathbf{\Delta}(\mathrm{d}c^N) \leqq \mathcal{I}(0, c_0) + \int_0^T \partial_t \mathcal{I}(t, \widetilde{c}^N(t))\,\mathrm{d}t, \tag{2.12}$$

where $\widetilde{c}^N(t) = c_{k-1}^N$ *for* $t \in [t_{k-1}, t_k)$ *is the right-continuous interpolant.*

The suitability of (IP) is also manifested in the fact that (2.12) can be improved to a two-sided estimated, see [MiT99, MiT02].

Proof. First we observe that the weak lower semicontinuity of $\mathcal{I}(t_k, \cdot)$ and the convexity of $\mathbf{\Delta}(\cdot - c_{k-1}^N)$ implies that the sum is weakly lower semicontinuous. The positivity of $\mathcal{I}$ implies coercivity such that for every $c \in \mathcal{P}$ with $\|c - c_k^N\| > C \cdot \mathcal{I}(t_{k+1}, c_k^N)$ we have

$$\mathcal{I}(t_{k+1}, c_k^N) \leqq \mathcal{I}(t_k, c_k^N) + \mathcal{I}(t_{k+1}, c) < \mathcal{I}(t_{k+1}, c) + \mathbf{\Delta}(c - c_k^N).$$

Therefore $\|c_{k+1}^N - c_k^N\| \leqq C \cdot \mathcal{I}(t_{k+1}, c_k^N)$ holds. The weak compactness (2.11) implies now the existence of solutions to (IP).

The stability of $c^N(t_k) = c_k^N$ arises from its minimizing property. We have

$$\begin{aligned}\mathcal{I}(t_k,a)+\mathbf{\Delta}(a-c_k^N) &= \mathcal{I}(t_k,a)+\mathbf{\Delta}(a-c_{k-1}^N)+\mathbf{\Delta}(a-c_k^N)-\mathbf{\Delta}(a-c_{k-1}^N)\\ &\geqq \mathcal{I}(t_k,c_k^N)+\mathbf{\Delta}(c_k^N-c_{k-1}^N)+\mathbf{\Delta}(a-c_k^N)-\mathbf{\Delta}(a-c_{k-1}^N)\\ &\geqq \mathcal{I}(t_k,c_k^N),\end{aligned}$$

where the triangle inequality (2.5) has been used for the last estimate. To obtain the discrete energy inequality we first observe that (2.12) is equivalent to

$$\sum_{k=1}^{N}\Big(\mathcal{I}(t_k,c^N(t_k))-\mathcal{I}(t_k,c^N(t_{k-1}))+\mathbf{\Delta}(c^N(t_k)-c^N(t_{k-1}))\Big)\leqq 0. \qquad (2.13)$$

From the fact that c_k^N minimizes $\mathcal{I}(t_k,\cdot)+\mathbf{\Delta}(\cdot-c_{k-1}^N)$ it follows that each term in (2.13) is nonpositive and hence (2.12) holds. □

It remains for us to consider under what condition the functions $c^N \in \mathrm{BV}([0,T],\mathcal{P})$ converge to a limit and whether this limit is an admissible process. The essential tool is a version of Helly's theorem for functions which take values in Banach spaces.

Theorem 2.7 ([BaP86] Thm. 3.5, Ch. 1**).** *Let X be a reflexive separable Banach space with separable dual X^*. Let $\{w_n\} \subset \mathrm{BV}([a,b];X)$ be such that $\|w_n(t)\| \leqq C$ for $t \in [a,b]$ and $\mathrm{Var}(w_n;[a,b]) \leqq C$ for all n. Then there exists a subsequence $\{w_{n_k}\} \subset \{w_n\}$ and a function $w \in \mathrm{BV}([a,b];X)$ such that, as $k \to \infty$, $w_{n_k} \rightharpoonup w(t)$ in X for all $t \in [a,b]$.*

Since in our application the Banach space equals $\mathrm{L}^1(\Omega,\mathbb{R}^n)$, we need a version without reflexivity of X and separability of X^*. Here we take advantage of the subset $\mathcal{P}$ and property (2.11). We have the following simple generalization.

Corollary 2.8. *Let X be a separable Banach space and $\mathcal{P} \subset X$ satisfy* (2.11)*. Then, for each bounded sequence $(c^N)_{N\in\mathbb{N}}$ in $\mathrm{BV}([0,T],X)$ there exists a subsequence N_k and a limit function $c^\infty \in \mathrm{BV}([0,T],\mathcal{P})$ such that $c^{N_k}(t) \rightharpoonup c^\infty(t)$ as $k \to \infty$ for all $t \in [0,T]$.*

Clearly the existence theorem, Theorem 2.6, provides a sequence (c^N) which is bounded in $\mathrm{BV}([0,T],X)$ and thus we can extract a limit $c^\infty \in \mathrm{BV}([0,T],\mathcal{P})$. From (2.12) it is not so difficult to show that c^∞ satisfies the weak energy inequality, hence it remains to check whether the process c^∞ is stable. There are two ways to derive stability: (i) if the convergence is not only weak, but strong, then the continuity of $\mathbf{\Delta}$ suffices to prove stability since $\mathcal{S}(t)$ is strongly closed; and (ii) if the set of stable states is weakly closed, then the stability of the weak limit follows. It is case (ii) which we will need for our application; hence we formulate it in the theorem below and refer to [MiT02] for more general cases.

Theorem 2.9. *Let the assumptions of Theorem 2.6 be satisfied. Assume further that*

$$\text{for all } t \in [0,T] \text{ the mapping } c \mapsto \partial_t \mathcal{I}(t,c) \text{ is weakly continuous} \tag{2.14}$$

and that for all $t \in [0,T]$ *the stable sets* $\mathcal{S}(t)$ *are weakly closed. Consider a sequence of hierarchical discretizations* (*specified in the proof*) *and let* c^∞ *be the limit as constructed above. Then,* $c = (c^\infty)^- \in \mathrm{BV}([0,T],\mathcal{P})$ *is an admissible process with* $c(0) = c_0$.

Proof. We have to show that the process c^∞ which is constructed in Theorem 2.6 satisfies the energy inequality and is stable. By the weak lower semicontinuity of $\mathcal{I}(t,\cdot)$ and $\mathbf{\Delta}$ and the weak continuity $\partial_t\mathcal{I}(t,\cdot)$ (cf. (2.14)) we find that the weak energy inequality (2.12) is stable under pointwise weak convergence, hence c^∞ satisfies the weak energy inequality (E). To show that $c = (c^\infty)^-$ also satisfies (E), we first note that the boundedness of the variation of c^∞ implies that the set $\{\, t \in [0,T] \mid c(t) \neq c^\infty(t) \,\}$ is at most countable, thus $\int_0^T \partial_t\mathcal{I}(t,c(t))\,\mathrm{d}t = \int_0^T \partial_t\mathcal{I}(t,c^\infty(t))\,\mathrm{d}t$. Together with $c(0) = c^\infty(0) = c_0$ and $\int_0^T \mathbf{\Delta}(\mathrm{d}c) \leqq \int_0^T \mathbf{\Delta}(\mathrm{d}c^\infty)$, this gives the result.

A sequence $(\Pi_r)_{r\in\mathbb{N}}$ of discretizations with $\Pi_r = \{t_0^{N_r}, t_1^{N_r}, \dots, t_{N_r}^{N_r}\}$ and $t_k^{N_r} < t_{k+1}^{N_r}$ is called hierarchical if $\{0,T\} \subset \Pi_r \subset \Pi_{r+1}$ and if the fineness $\Phi(\Pi_r) = \max\left\{ t_k^{N_r} - t_{k-1}^{N_r} \mid k = 1,\dots,N_r \right\}$ of Π_r tends to 0. Let $\mathcal{T} = \cup_{r\in\mathbb{N}}\Pi_r$, then $\mathcal{T}$ is dense in $[0,T]$ and for each $t \in \mathcal{T}$ we have $c^{N_r}(t) \in \mathcal{S}(t)$ for all sufficiently large r. By the weak convergence to $c^\infty(t)$ and the weak closedness of $\mathcal{S}(t)$ we obtain $c^\infty(t) \in \mathcal{S}(t)$ for all $t \in \mathcal{T}$. Using Lemma 2.4 we conclude that $c = (c^\infty)^-$ is a stable process. □

In particular, for $\mathcal{I}(t,c) = \widetilde{\mathcal{I}}(c) - \langle G(t), c\rangle$ with $G \in \mathrm{C}^1([0,T], X^*)$ the assumption (2.14) is satisfied.

3. Application to martensitic phase transformations

In this section we will demonstrate that the hysteretic response of shape-memory alloys can be modeled within the framework of rate-independent evolution problems. It turns out that finding a suitable linear structure (the Banach space X) on the state space is a nontrivial problem. The expressions for both the potential and the dissipated energy are only obvious in the case of pure phase distributions, therefore we indicate that the energies are only defined on pure phase distributions by adding a superscript $^{\mathrm{p}}$. Instead of assuming a dissipation rate $\mathbf{\Delta}$ we give an expression for the minimal dissipation $\mathcal{D}^{\mathrm{p}}(c_1^{\mathrm{p}}, c_2^{\mathrm{p}})$ which occurs when a state c_1^{p} is transformed into c_2^{p}. Extending the energies to linear combinations of pure phase distributions means that a mixture theory has to be constructed where also concentrations can be treated correctly. This step is postponed to the next section.

3.1. Modeling hysteresis via metastability or via internal variables

Before starting with the PT problem we relate the above model to the general theory of systems with hysteretic behavior. Hysteresis is a well-known effect which is either attributed to rate-independent friction (like dry friction) or to metastability in nonlinear systems. We want to show that there is a close connection between both situations when we consider slow or quasistatic processes, their extreme being rate-independent processes which are considered here. In particular, we demonstrate how the usage of internal variables enables us to use global minimization instead of studying local stability.

We show this connection for a simple model with a mass point moving slowly (without inertia) in the nonconvex potential

$$E(t,w) = \rho(w) - g(t)w \quad \text{with } \rho(w) = \tfrac{1}{4}(w^2-3)^2,$$

where $g : [0,T] \to \mathbb{R}$ is the slowly varying loading. Since the position $w(t) \in \mathbb{R}$ of the mass point always minimizes $E(t,\cdot)$ locally, we have $\rho'(w(t)) = g(t)$ and $\rho''(w(t)) \geqq 0$, which may have no or one solution lying in $(-\infty,-1]$ or $[1,\infty)$, respectively. The first situation is called phase e_1 and the second is called phase e_2. We assume that the mass point remains in a locally stable state (metastable) as long as possible. If stability is lost, then it drops into the nearest stable point. The energy loss will be dissipated.

Now take $g(t) = \min\{t-2, 8-t\}$, $t \geqq 0$, and $w(0) = -2$. Then $\rho'(w(t)) = g(t)$ with $w(t) \leqq -1$ for $t \in [0,4] \cup (10,\infty)$ and $w(t) \in [1,\infty)$ for $t \in (4,10]$. Hence there is a sudden phase change at $t = 4$ (with $g(t) = 2$) from e_1 to e_2 where w jumps from -1 to 2 and the energy drops down from 3 down to $-15/4$. At $t = 10$ (with $g(t) = -2$) the phase changes back from e_2 to e_1 where w jumps from 1 to -2 and the energy drops again from 3 to $-15/4$. (Note that the global minimizer changes at $g(t) = 0$ without any energy loss; this relates to the Maxwell line having no hysteresis.)

The same hysteresis effect can be obtained by using the internal variable $c^{\mathrm{p}} \in \{e_1, e_2\}$ and the dissipation coefficients $\kappa_{1\to 2} = \kappa_{2\to 1} = 3-(-15/4) = 27/4$. We choose a strictly convex function $\widehat{\rho} : \mathbb{R} \to \mathbb{R}$ with $\widehat{\rho}(w) = \rho(w)$ for $w \leqq -1$ and define

$$\widetilde{E}(t,w,c^{\mathrm{p}}) = \begin{cases} \widehat{\rho}(w) - g(t)w & \text{for } c^{\mathrm{p}} = e_1, \\ \widehat{\rho}(-w) - g(t)w & \text{for } c^{\mathrm{p}} = e_2; \end{cases}$$

and $D^{\mathrm{p}} : P^{\mathrm{p}} \times P^{\mathrm{p}} \to \mathbb{R}_{\geqq}$ with $\kappa_{i\to j}$ as above. Then, $(w(t), c^{\mathrm{p}}(t))$ is stable if

$$\widetilde{E}(t,w(t),c^{\mathrm{p}}(t)) \leqq \widetilde{E}(t,\widehat{w},a^{\mathrm{p}}) + D^{\mathrm{p}}(c^{\mathrm{p}}(t),a^{\mathrm{p}}) \ \text{ for } \widehat{w} \in \mathbb{R},\ a^{\mathrm{p}} \in \{e_1,e_2\}.$$

Using $a^{\mathrm{p}} = c^{\mathrm{p}}(t) = e_j$ we obtain the necessary local criterion $\widehat{\rho}'(w(t)) = g(t)$ which gives a unique solution $w_{g(t)}$ by strict convexity. Let $\eta(g) = \widehat{\rho}(w_g) - gw_g = \min\{\widehat{\rho}(w) - gw \mid w \in \mathbb{R}\}$; then $-\eta(\cdot)$ is the Legendre transform of $\widehat{\rho}$ with $\eta(2) = 3$ and $\eta(-2) = -15/4$. Additionally, we may assume, by choosing $\widehat{\rho}$ suitably for $w > 1$, that $\eta(g) < 27/4 + \eta(-g)$ for $g > 2$. Now, asking for stability of

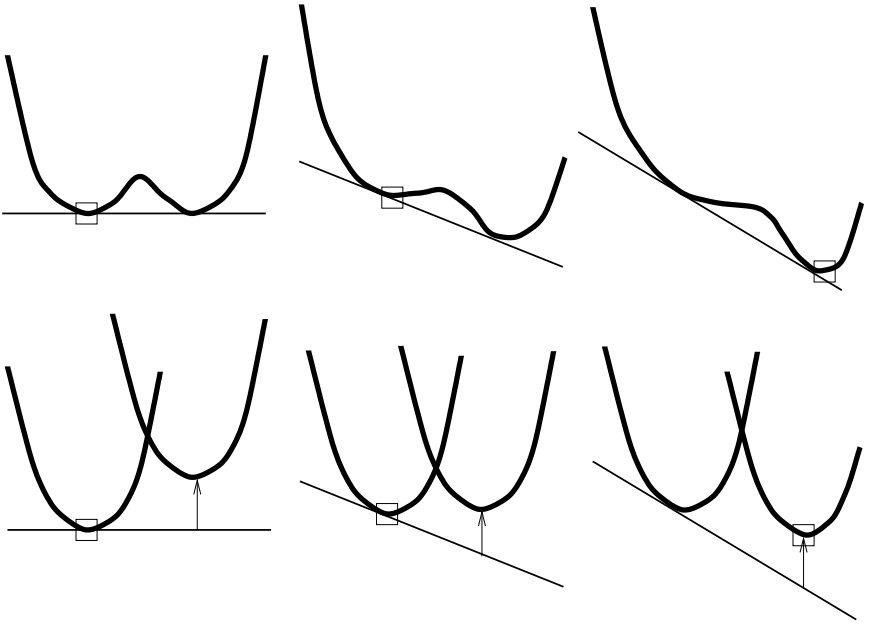

Fig. 3.1. The upper three graphs show $E(t,\cdot)$ for the three time levels $t = 2$, $t = 3.8$ and $t = 4.2$ (from left to right). The lower graphs display $\widetilde{E}(t,\cdot,c^{\mathrm{p}})$ with $c^{\mathrm{p}} = e_1$ to the right and $c^{\mathrm{p}} = e_2$ to the left for the same time levels. The squares $\square$ indicate the (meta) stable positions.

$(w(t), c^{\mathrm{p}}(t)) = (w_{g(t)}, e_1)$ with respect to $(\widehat{w}, e_2)$, we find the additional restriction $\eta(g(t)) \leqq 15/4 + \eta(-g(t))$ which by construction is equivalent to $g(t) \leqq 2$.

Thus, using the same loading $g(t) = \min\{t-2, 8-t\}$, $t \geqq 0$, as above and the initial condition $w(0) = -2$, we obtain exactly the same solution $w(t)$ if we additionally set $c^{\mathrm{p}}(t) = e_1$ for $t \in [0,4] \cup (10,\infty)$ and $c^{\mathrm{p}}(t) = e_2$ for $t \in (4,10]$. The major difference to the approach without an internal variable is that in this situation the solution pair $(w(t), c^{\mathrm{p}}(t))$ is a global minimizer of $\widetilde{E}(t,\cdot,\cdot) + D(c^{\mathrm{p}}(t),\cdot)$ whereas $w(t)$ alone is only a local minimizer of $E(t,\cdot)$.

3.2. Mathematical formulation of the PT model

We return to the PT model and denote by $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, the reference configuration of an elastically deformable body. For $n > 1$ the discrete set $P^{\mathrm{p}} = \{e_1, \ldots, e_n\}$ is the set of possible *pure phases*, e_j is the j-th unit vector in $\mathbb{R}^n$. The purpose of this notation is to identify a very natural relaxation with the convexification of $\mathcal{P}$ in the following section. The set $\mathcal{P}^{\mathrm{p}} = \mathrm{L}^1(\Omega, P^{\mathrm{p}})$ is the set of pure states; the superscript $^{\mathrm{p}}$ is needed to distinguish between unrelaxed (or pure-phase) models and relaxed models where c takes its values in a continuous set.

The elastic material properties of phase e_j are determined by the stored-energy density $W_{e_j}(F)$ where F replaces the deformation gradient ∇u. For given state

$c^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$ and deformation field $u : \Omega \to \mathbb{R}^d$ the elastic bulk energy is given by

$$\mathcal{E}^{\mathrm{p}}_{\mathrm{elast}}(c^{\mathrm{p}}, u) = \int_\Omega W_{c^{\mathrm{p}}(x)}(x, \nabla u(x))\,\mathrm{d}x.$$

Throughout the paper we will assume that the energy-density functions W_{e_i} satisfy the following standard assumptions of elasticity:

(i) *Growth conditions:* there exist $C > 0$ and $1 < p \leqq q < \infty$ such that

$$|F|^p/C - C \leqq W_{e_i}(F) \leqq C|F|^q + C \text{ for all } F \in \mathbb{R}^{d\times d}; \tag{3.1}$$

(ii) $W_{e_i}(\cdot)$ is *quasiconvex*, i.e., for all $F \in \mathbb{R}^{d\times d}$ and all $\varphi \in C_0^\infty((0,1)^d)$ we have

$$W_{e_i}(F) \leqq \int_{(0,1)^d} W_{e_i}(F + \nabla\varphi(y))\,\mathrm{d}y. \tag{3.2}$$

These assumptions are needed to guarantee that the elastic problem has a solution. This means that is is possible to find a minimizer to $\mathcal{E}^{\mathrm{p}}_{\mathrm{elast}}(c^{\mathrm{p}}, \cdot)$ where the state c^{p} is kept fixed. Although the existence of minimizers is not really required in our theory, it is a typical assumption for any realistic choice of W_{e_i}. Our growth assumptions exclude true energy-density functions for nonlinear elasticity which should satisfy $W_{e_i}(F) = +\infty$ for all F with $\det F \leqq 0$. At present the analysis for this case is not understood but the general methodology of our modeling procedure still works. Our application in Section 5 is for linearized elasticity where (3.1) holds with $q = p = 2$.

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 (affine) subspace $\mathcal{V}$ of $\mathrm{W}^{1,p}(\Omega)$. Without going into the details we assume that the change of the Neumann-boundary data and the bulk force can be represented by a time-dependent functional $G : [0, T] \to \mathcal{V}^*$, the dual space of $\mathcal{V}$. Thus, at time t the system is described by $(c^{\mathrm{p}}, u) \in \mathcal{P}^{\mathrm{p}} \times \mathcal{V}$ and has the total energy (Gibbs' energy)

$$\mathcal{E}^{\mathrm{p}}(t, c^{\mathrm{p}}, u) = \int_\Omega W_{c^{\mathrm{p}}(x)}(\nabla u(x))\,\mathrm{d}x - \langle G(t), u\rangle.$$

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

We assume that each PT leads to a dissipation of an amount of energy which is proportional to the volume of the region occupied by the transformed material times the constant $\kappa_{i\to j}$ depending only on the phase e_i before and the phase e_j after the PT. Since the dissipated energy should be positive and finite we have $\kappa_{i\to j} \geqq 0$ and $\kappa_{i\to i} = 0$ for every i, j. The general theory requires that $\mathbf{\Delta}$ is coercive and convex. These two requirements translate directly into

$$\textit{coercivity:} \qquad \kappa_{i\to j} > 0 \text{ if } i \neq j, \tag{3.3}$$

$$\textit{triangle inequality:} \qquad \kappa_{i\to j} \leqq \kappa_{i\to k} + \kappa_{k\to j} \tag{3.4}$$

for every i, j, k. Note that our state space $\mathcal{P}^{\mathrm{p}}$ is not endowed with a linear structure since phase-distribution functions cannot be multiplied with a scalar. With these assumptions we can postulate our dissipation function which instead of taking rates as an argument is defined on pairs of states.

$$\mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}(t_1), c^{\mathrm{p}}(t_2)) = \int_\Omega D^{\mathrm{p}}(c^{\mathrm{p}}(t_1, x), c^{\mathrm{p}}(t_2, x))\,\mathrm{d}x \quad \text{where } D^{\mathrm{p}}(e_i, e_j) = \kappa_{i\to j}.$$

Consequently the total dissipation associated with a process is given by the sum of the individual dissipations:

$$\mathrm{Diss}^{\mathrm{p}}(c^{\mathrm{p}}; t_1, t_2) = \sup\left\{ \sum_{k=1}^{m} \mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}(\tau_{k-1}), c^{\mathrm{p}}(\tau_k)) \;\middle|\; m\in\mathbb{N}, \right.$$
$$\left. t_1 \leqq \tau_0 < \tau_1 < \ldots < \tau_m \leqq t_2 \right\}.$$

The central concept which determines the evolution of the internal state c^{p} and the deformation u is the stability criterion (S) which is derived from the postulate of realizability in [Lev95, Lev97]. Using the notation introduced so far, it reads

$$\mathcal{E}^{\mathrm{p}}(t, c^{\mathrm{p}}, u) \leqq \mathcal{E}^{\mathrm{p}}(t, b^{\mathrm{p}}, v) + \mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}(t), b^{\mathrm{p}}) \tag{3.5}$$

for all $b^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$, $v \in \mathcal{V}$. Since the dissipated energy $\mathcal{D}^{p}$ does not depend on the deformation u, the concept of stability implies that for given t and c^{p} the deformation u is a global minimizer of $\mathcal{E}$. Hence, we introduce the energy of a state c^{p} via

$$\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}) = \inf\left\{ \mathcal{E}^{\mathrm{p}}(t, c^{\mathrm{p}}, v) \;\middle|\; v \in \mathcal{V} \right\}.$$

In analogy to (S) and (E) we say that a process $c^{\mathrm{p}} : [0, T] \to \mathcal{P}^{\mathrm{p}}$ is *stable* if

$$\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}(t)) \leqq \mathcal{I}^{\mathrm{p}}(t, a^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}(t), a^{\mathrm{p}}) \quad \text{for } a^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}},\ t \in [0, T] \tag{3.6}$$

and it satisfies the *energy inequality* if

$$\mathcal{I}^{\mathrm{p}}(t_2, c^{\mathrm{p}}(t_2)) + \mathrm{Diss}^{\mathrm{p}}(c^{\mathrm{p}}; t_1, t_2) \leqq \mathcal{I}^{\mathrm{p}}(t_1, c^{\mathrm{p}}(t_1)) - \int_{t_1}^{t_2} \langle \dot{G}(t), u(t)\rangle\,\mathrm{d}t \tag{3.7}$$

for $0 \leqq t_1 < t_2 \leqq T$. Here the last term contains the energy contribution of the work done by the external loading. A process is called *admissible for $\mathcal{I}^{\mathrm{p}}$ and $\mathcal{D}^{\mathrm{p}}$* if it is stable and satisfies the energy inequality.

The definition of stability gives a time-dependent restriction for $c^{\mathrm{p}}(t) \in \mathcal{P}^{\mathrm{p}}$. It does not see the (rate-independent) dynamics of the process. The stability implies that for no time t_1 can the process be changed on $(t_1, t_2]$ such that the difference between dissipation and energy gain is negative. Similarly, the energy inequality generates a restriction in the space of stresses and strain rates. The term $\mathrm{Diss}^{\mathrm{p}}(c^{\mathrm{p}}; t_1, t_2)$ includes the dissipation which occurs through phase transformations in the time interval $[t_1, t_2]$. Note that the analogue of Theorem 2.5 holds also for admissible processes in this generalized sense. For instance, by stability, at time t a PT from $c^{\mathrm{p}}_{\mathrm{old}}$ to $c^{\mathrm{p}}_{\mathrm{new}}$ is possible only when the gain in the energy $\mathcal{I}^{\mathrm{p}}$ is at

least as large as the associated dissipation. However, the energy inequality gives the opposite estimate which implies that at a jump we must satisfy the equality $\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}_{\mathrm{old}}) - \mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}_{\mathrm{new}}) \geqq \mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}_{\mathrm{old}}, c^{\mathrm{p}}_{\mathrm{new}})$.

Until now, our model does not quite fit into the abstract framework outlined in Section 2 since we have not specified a Banach space X. The sets on which the energies are defined do not have any linear structure yet. This step will be completed only in the following section where the question, of how to derive a relaxed model, will be discussed more seriously. Nevertheless, the definition of admissibility leads to the following *time-continuous problem*.

(CP) For given $c^{\mathrm{p}}_0 \in \mathcal{P}^{\mathrm{p}}$, find an admissible $c^{\mathrm{p}} : [0, T] \to \mathcal{P}^{\mathrm{p}}$ with $c^{\mathrm{p}}(0) = c^{\mathrm{p}}_0$.

It is not obvious that the set of stable states is nonempty. In [The01] it is proved that, if $(\mathcal{P}^{\mathrm{p}}, \mathcal{D}^{\mathrm{p}})$ forms a complete metric space, then stable states exist. The martensitic system satisfies this condition. To actually find stable states, i.e., states which are relevant for the evolution, it is possible to derive necessary local conditions in the case of the martensitic system. For a proof of the following two results we refer to [MTL98]. Result (i) can be interpreted as the stability condition of a pure phase e_i with respect to formation of a nucleus including different phases with average c. This result shows that already stability is intrinsically linked to the relaxed density functions $\mathbb{W}$ and Δ obtained in Sections 4.2 and 4.3. Result (ii) relates to stability of (smooth) interfaces, see the discussion below.

Theorem 3.1. (i) *Let $c^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$ be stable and let $x_0 \in \Omega$ be such that c^{p} and $F = \nabla u$ are continuous at $x = x_0$. Then, with $\mathbb{W}(a, F)$ and Δ from* (4.5) *and* (4.10),

$$W_{c^{\mathrm{p}}(x_0)}(F(x_0)) \leqq \Delta(a - c(x_0)) + \mathbb{W}(a, F(x_0)) \quad \text{for all } a \in P = \mathrm{conv}(P^{\mathrm{p}}).$$

(ii) *Let $c^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$ be stable and let $x_0 \in \Omega$ be a point where c^{p} has a phase boundary with normal vector ν. Let $(e^{\pm}, F^{\pm})$ be the left and right limits of $(c^{\mathrm{p}}(x), F(x))$ which satisfy by strain and stress compatibility $F^+ - F^- = a \otimes \nu$ and $T_0 \stackrel{\mathrm{def}}{=} \partial_F W_{e^+}(F^+)\nu = \partial_F W_{e^-}(F^-)\nu$. Then,*

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

The scalar quantity $\xi = W_{e^-}(F^-) - W_{e^+}(F^+) + T_0 \cdot ([F^+ - F^-]\nu)$ is the normal component $\nu \cdot (E_0 \nu)$ of the Eshelby tensor E_0. It is well known in the literature [Gri91, KaR88, Lev95, Lev97] and is frequently denoted as the driving force for the interface. As long as ξ lies strictly between $-D^{\mathrm{p}}(e^+, e^-)$ and $D^{\mathrm{p}}(e^-, e^+)$ the interface cannot move in a time-continuous process since the dissipation plays the role of a threshold. If ξ reaches the value $D^{\mathrm{p}}(e^-, e^+)$ the interface can move such that phase e^+ grows, and analogously phase e^- will start to grow if $\xi = -D^{\mathrm{p}}(e^+, e^-)$.

From the abstract theory in Section 2, especially the incremental approach in Section 2.3, it is natural to try to find solutions by time discretization. Choosing a discrete set of times $0 = t_0 < t_1 < \cdots < t_k < \cdots < t_N = T$ we are lead to consider the associated *incremental problem* (IP):

(IP) For given $c_0^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$, find $c_1^{\mathrm{p}}, \dots, c_N^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$ such that

$$\mathcal{I}^{\mathrm{p}}(t_k, c_k^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_{k-1}^{\mathrm{p}}, c_k^{\mathrm{p}}) = \inf \left\{ \mathcal{I}^{\mathrm{p}}(t_k, a^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_{k-1}^{\mathrm{p}}, a^{\mathrm{p}}) \mid a^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}} \right\},$$

for $k = 1, \dots, N$.

In contrast to Section 2 we do not have the special form $\mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}}) = \mathbf{\Delta}(c^{\mathrm{p}} - a^{\mathrm{p}})$. However, the triangle inequality (3.4) takes over the role of convexity in Section 2 and we are still able to conclude that the solutions of (IP) are stable for $t = t_1, \dots, t_N$. In complete analogy to the abstract theorem, Theorem 2.6, we obtain the desired properties for solutions of (IP).

Lemma 3.2. *Assume that* $D^{\mathrm{p}} : P^{\mathrm{p}} \times P^{\mathrm{p}} \to \mathbb{R}_{\geqq}$ *satisfies* (3.4)*, then solutions of* (IP) *are stable, i.e.,* $\mathcal{I}^{\mathrm{p}}(t_k, c_k^{\mathrm{p}}) \leqq \mathcal{I}^{\mathrm{p}}(t_k, a^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_k^{\mathrm{p}}, a^{\mathrm{p}})$ *for all* $a^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$*, and satisfy the discrete energy inequality*

$$\mathcal{I}^{\mathrm{p}}(t_k, c_k^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_{k-1}^{\mathrm{p}}, c_k^{\mathrm{p}}) \leqq \mathcal{I}^{\mathrm{p}}(t_{k-1}, c_{k-1}^{\mathrm{p}}) + \int_{t_{k-1}}^{t_k} \partial_t \mathcal{I}^{\mathrm{p}}(s, c_{k-1}^{\mathrm{p}}) \, \mathrm{d}s.$$

We refer to Remark 4.8 for the necessity of the triangle inequality in this context.

4. Coarse graining via relaxation

The formulation we derived so far is not satisfactory, for two reasons:

(1) The existence of admissible processes cannot be assured, not even for the incremental problem. Since the state space $\mathcal{P}^{\mathrm{p}} = \mathrm{L}^1(\Omega, P^{\mathrm{p}})$ is *not* weakly closed, it is unclear whether for fixed $t \in [0, T]$ and $a^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$, the functional

$$c^{\mathrm{p}} \mapsto \mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}})$$

has minimizers. Therefore we cannot use the incremental problem to construct solutions.

(2) The numerical solution of the incremental problem would exhibit strong oscillations, cf. [CaP97]. Energy considerations show that if the data is chosen in order to achieve deformations in the "soft" directions of a shape-memory alloy, strong oscillations are needed to avoid large stresses.

For these two reasons it is necessary to derive a coarse-grained model which relies on effective quantities like phase portions instead of being restricted to pure phase distributions. It is not particularly difficult to find extensions from pure-phase models to models with phase mixtures so that the existence of admissible processes can be guaranteed. The problem is to establish a clear link between the extended and the original model. Such links can be obtained in several ways. An abstract notion which is closely related to the spirit of Γ-convergence can be found in [The01]. Here we develop an approach based on the incremental method which is used to construct solutions. We first introduce the notion of separate relaxation which is based only on phase portions and compare it then to a more sophisticated definition (incremental relaxation).

Since existence and uniqueness of a separately relaxed model (not the solution!) is obvious, we can study its properties in the following sections. First, we derive more explicit expressions for the separately relaxed energies. Then we explain, how these formulas can be used to convert the rather unusual incremental problem into a standard problem in the context of nonlinear elasticity theory.

Finally we show that the special form of the separate relaxation allows us to deduce a simple differential inclusion as a necessary condition for relaxed admissible processes with respect to the separately relaxed energies.

For each notion of relaxation we obtain a new incremental problem and rate-independent evolution problem. To distinguish all these objects properly we have tabled the relevant nomenclature.

	unrelaxed PT problem	separate relaxation	incremental relaxation
states, energy, diss.	$\mathcal{P}^{\mathrm{p}}, \mathcal{I}^{\mathrm{p}}, \mathcal{D}^{\mathrm{p}}$	$\mathcal{P}, \mathcal{I}, \mathcal{D}$	$\mathcal{P}, \mathcal{I}, \mathcal{D}$
continuous problem	(CP)	(SRCP)	
incremental problem	(IP)	(SRIP) (SRIP)′	(RIP)

4.1. Two notions of relaxation

Here we describe two possible notions of relaxation which remain solely on the level of the incremental problem (IP). Since (IP) is a variational problem we may study its relaxation. Neither in a real physical process nor in a mathematical approximation of (IP) can we expect exact minimization of $\mathcal{I}^{\mathrm{p}}(t_k, \cdot) + \mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}_{k-1}, \cdot)$ to occur. The general philosophy of relaxation of rate-independent problems is developed in [The01, Mi02b].

4.1.1. Separate relaxation. The simplest approach, which has been successfully applied in related situations (cf. [FrM93]), consists in relaxing the functional $\mathcal{J}^{\mathrm{p}}(t, a^{\mathrm{p}}, c^{\mathrm{p}}) = \mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}})$. The special structure of $\mathcal{J}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}})$, namely that it is a sum of two terms, simplifies the analysis enormously. The first term $\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}})$ does not depend on a^{p} and the second term $\mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}})$ depends on a^{p} and c^{p} only pointwise under the integral over Ω.

We define $\mathcal{P}$ as the weak closure of $\mathcal{P}^{\mathrm{p}}$; obviously $\mathcal{P} = \mathrm{L}^1(\Omega, P)$ where P is the convex hull of P^{p}, the unit simplex. For $a, c \in \mathcal{P}$ we now define the relaxations

$$\mathcal{I}(t, c) = \inf \left\{ \liminf_{m\to\infty} \mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}_m) \mid c^{\mathrm{p}}_m \rightharpoonup c \text{ for } m \to \infty \right\}, \tag{4.1}$$

$$\mathcal{D}(a, c) = \inf \left\{ \liminf_{m\to\infty} \mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}_m, c^{\mathrm{p}}_m) \mid a^{\mathrm{p}}_m \rightharpoonup a,\ c^{\mathrm{p}}_m \rightharpoonup c \text{ for } m \to \infty \right\}, \tag{4.2}$$

$$\mathcal{J}_k(a, c) = \mathcal{I}(t_k, c) + \mathcal{D}(a, c).$$

Note that $\mathcal{D}^{\mathrm{p}}(\cdot, \cdot)$ is relaxed in both variables simultaneously. It is not so difficult to see that $\mathcal{J}_k$ is in fact the simultaneous relaxation of $\mathcal{J}^{\mathrm{p}}_k$ in both its arguments, viz.,

$$\mathcal{J}_k(a, c) = \inf \left\{ \liminf_{m\to\infty} \mathcal{J}^{\mathrm{p}}_k(a^{\mathrm{p}}_m, c^{\mathrm{p}}_m) \mid a^{\mathrm{p}}_m \rightharpoonup a,\ c^{\mathrm{p}}_m \rightharpoonup c \text{ for } m \to \infty \right\}.$$

It is a triviality that the separately relaxed incremental problem (SRIP) has a solution:

(SRIP) For given $c_0^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$, find $c_1, \ldots, c_N \in \mathcal{P}$ such that

$$\mathcal{J}_k(c_{k-1}, c_k) = \inf \{ \mathcal{J}_k(c_{k-1}, a) \mid a \in \mathcal{P} \}.$$

Proposition 4.1. *For all $c_0 \in \mathcal{P}$ the sequence of minimization problems* (SRIP) *has a solution.*

This approach is obviously too simplistic to be helpful in situations where not only the concentration but also more delicate properties of the microstructure play a role. However, because of the concreteness of the notion of separate relaxation (only phase portions occur), it is possible to obtain structural results on $(\mathcal{I}, \mathcal{D}, \mathcal{P})$. In Sections 4.2 and 4.3 we will derive formulas for both $\mathcal{I}$ and $\mathcal{D}$ which are still local in space.

The notion of separate relaxation is quite closely related to similar approaches for stationary problems. Obviously, it is uniquely determined by the unrelaxed problem. Its main value for the relaxation of rate-independent evolution problems is that it leads to well-posed incremental problems and provides good candidates for an incrementally compatible relaxation.

4.1.2. Incremental relaxation. To find a more honest notion of relaxation we have to take the influence of the microstructure into account. An attempt which avoids discussing the structure of the time-continuous evolution problems is given by the following *approximate incremental problem* $(\mathrm{AIP})_\varepsilon$ where quasiminimal solutions are allowed.

$(\mathrm{AIP})_\varepsilon$ For given $\varepsilon > 0$ and $c_0^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$, find $c_1^{\mathrm{p}}, \ldots, c_N^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$ such that

$$\mathcal{I}^{\mathrm{p}}(t_k, c_k^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_{k-1}^{\mathrm{p}}, c_k^{\mathrm{p}}) \leqq \varepsilon + \inf \left\{ \mathcal{I}^{\mathrm{p}}(t_k, a^{\mathrm{p}}) + \mathcal{D}^{\mathrm{p}}(c_{k-1}^{\mathrm{p}}, a^{\mathrm{p}}) \middle| a^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}} \right\}.$$

Clearly, this problem always has (many) solutions $(c_{1,\varepsilon}^{\mathrm{p}}, \ldots, c_{N,\varepsilon}^{\mathrm{p}})$. It is not at all clear under what conditions the limits $\varepsilon \to 0$ and $N \to \infty$ commute. Here we propose a relaxation which is based on the incremental problem, consequently we first send ε to 0.

Definition 4.2. Let X be a Banach space and let $(\mathcal{I}, \mathcal{D}, \mathcal{P})$ be an extension of $(\mathcal{I}^{\mathrm{p}}, \mathcal{D}^{\mathrm{p}}, \mathcal{P}^{\mathrm{p}})$ in the sense that $\mathcal{P}^{\mathrm{p}} \subset \mathcal{P} \subset X$, $\mathcal{I}|_{\mathcal{P}^{\mathrm{p}}} = \mathcal{I}^{\mathrm{p}}$ and $\mathcal{D}|_{\mathcal{P}^{\mathrm{p}} \times \mathcal{P}^{\mathrm{p}}} = \mathcal{D}^{\mathrm{p}}$. The incremental problem associated with $(\mathcal{I}, \mathcal{D}, \mathcal{P})$ is denoted by (RIP). Then, $(\mathcal{I}, \mathcal{D}, \mathcal{P})$ is called an *incremental relaxation* of $(\mathcal{I}^{\mathrm{p}}, \mathcal{D}^{\mathrm{p}}, \mathcal{P}^{\mathrm{p}})$ if

(i) for each $c_0 \in \mathcal{P}$ (RIP) has a solution,
(ii) $\mathcal{P}^{\mathrm{p}}$ is dense in $\mathcal{P}$ with respect to the weak topology, and
(iii) for any solution $(c_1, \ldots, c_N)$ of (RIP) there exist solutions $(c_{1,\varepsilon}^{\mathrm{p}}, \ldots, c_{N,\varepsilon}^{\mathrm{p}})$ of $(\mathrm{AIP})_\varepsilon$ such that $c_{k,\varepsilon}^{\mathrm{p}} \rightharpoonup c_k$ for $\varepsilon \to 0$.

An alternative (or additional) condition to (iii), which is probably much stronger, is that all weak limits of solutions of $(\mathrm{AIP})_\varepsilon$ are solutions of (RIP):

(iv) If $(c^{\mathrm{p}}_{1,\varepsilon}, \dots, c^{\mathrm{p}}_{N,\varepsilon})$ solves $(\mathrm{AIP})_\varepsilon$ and $c^{\mathrm{p}}_{k,\varepsilon} \rightharpoonup c_k$, then $(c_1, \dots, c_N)$ solves (RIP).

A natural question is: Which conditions guarantee that the separate relaxation indeed is an incremental relaxation? This problem can be understood best by considering infinimizing sequences $(c^{\mathrm{p}}_{k,\varepsilon})$ obtained from $(\mathrm{AIP})_\varepsilon$ with weak limits c_k for $\varepsilon \to 0$. The separate relaxation is based on the assumption

$$\mathcal{D}^{\mathrm{p}}(c^{\mathrm{p}}_{k-1,\varepsilon}, c^{\mathrm{p}}_{k,\varepsilon}) \to \mathcal{D}(c_{k-1}, c_k) \text{ for } \varepsilon \to 0. \tag{4.3}$$

Clearly this is not correct for general sequences. The problem is that the weak limits c_k only contain information on the macroscopic volume fractions of the pure phases and none on their microscopic arrangements. On the one hand, for infinimizing sequences the modeling error may be small as these sequences try to minimize $\mathcal{D}^{\mathrm{p}}$ which means that changes in the microscopic arrangement are energetically less favorable. Yet, on the other hand the microscopic arrangements are enforced by the first term $\mathcal{I}^{\mathrm{p}}(t_k, \cdot)$ and might differ at t_{k-1} and t_k. Then our relaxation underestimates the dissipated energy.

So far, a rigorous connection between (IP) and (SRIP) via $(\mathrm{AIP})_\varepsilon$ is only known in the (trivial) one-dimensional case and in the case of linearized elasticity with two phases with the same elastic moduli. The latter case is stated in the following theorem, a proof is found in [The00, The01].

Theorem 4.3. *Assume that* $n = 2$, $\mathbf{C} \in \mathrm{Lin}(\mathbb{R}^{d\times d}_{\mathrm{sym}}, \mathbb{R}^{d\times d}_{\mathrm{sym}})$ *is positive definite and that*

$$W_{e_i}(F) = \tfrac{1}{2}[\mathbf{C}(E-A_i)]:[E-A_i] + \beta^{(i)} \text{ with } A_i \in \mathbb{R}^{d\times d}_{\mathrm{sym}},\ \beta^{(i)} \in \mathbb{R}, \tag{4.4}$$

where $E = (F+F^T-2I)/2$. *Then the separate relaxation is an incremental relaxation in the sense of Definition 4.2.*

The main reason why this special case can be handled is that here the formation of microstructure can be controlled very well. It is sufficient to study lamination in one specific direction $\omega \in \mathbb{R}^d$. Moreover, it is exactly this two-phase problem for which we are able to provide an existence result for the associated time-continuous relaxed problem (SRCP), see Theorem 5.1.

4.2. Relaxation of the energy $\mathcal{I}^{\mathrm{p}}$

We recall that the energy-density functions $W_{e_i} : \mathbb{R}^{d\times d} \to \mathbb{R}$ of the pure phases are always assumed to be quasiconvex, cf. (3.2). To understand the idea of coarse graining we consider a small ball $B(x_0, r) = \{ x \in \Omega \mid |x-x_0| < r \}$ inside the body Ω where the averaged phase distribution is given by $c = \fint_{B(x_0,r)} c^{\mathrm{p}}(x)\,\mathrm{d}x$. We now allow for suitable rearrangements $c^{\mathrm{p}} \in \mathrm{L}^1(B(x_0, r), P^{\mathrm{p}})$ of the phases without changing the average and we also allow for fluctuations ϕ of the deformation which have to vanish on the boundary of the ball. For small r, these fluctuations can

be understood as microscopic adjustments which do not affect the macroscopic deformation. Letting $x = x_0 + ry$ with $y \in B$ we are led to the *mixture function*

$$\mathbb{W}(c, F) \stackrel{\text{def}}{=} \inf \left\{ \fint_B W_{c^{\mathrm{p}}(y)}(F + \nabla\phi(y))\,\mathrm{d}y \;\middle|\; \phi \in \mathrm{W}_0^{1,p}(B), \right.$$
$$\left. c^{\mathrm{p}} \in \mathrm{L}^1(B, P^{\mathrm{p}}),\ \fint_B c^{\mathrm{p}}(y)\,\mathrm{d}y = c \right\}. \tag{4.5}$$

This defines a function $\mathbb{W} : P \times \mathbb{R}^{d\times d} \to \mathbb{R}$; $(c, F) \mapsto \mathbb{W}(c, F)$ which satisfies $\mathbb{W}(e_j, F) = W_{e_j}(F)$ since W_{e_j} was assumed to be quasiconvex. Thus, $\mathbb{W}$ contains information on the mixture theory without the addition of new mechanics, just using the fact that elasticity theory is scale invariant. In general the minimum $\mathbb{W}(c, F)$ is not achieved, but we need an infimizing sequence $(c^{\mathrm{p}}_\varepsilon)_{\varepsilon>0}$; this tells us that certain microstructures are needed to minimize the energy under given phase fractions.

The functions $\mathbb{W}$ was already defined in [Koh91] as a tool to study the quasiconvexification of $\min\left\{ W_{e_j}(F) \mid j = 1, \dots, n \right\}$. There, $\mathbb{W}(c, F)$ itself plays a central role and is called the *quasiconvexification with fixed phase fractions*, denoted by $Q_c W(F)$. Related applications in the theory of phase transformations for shape-memory alloys are given in [Mie00, GMH02, Mi02b]. More recently the function appeared in [FKP94, LeR00] to model elastic materials with internal variables. In the latter work the function $\mathbb{W}$ is called *cross–quasiconvexification*.

The importance of the mixture function is that it is exactly the right tool to characterize the relaxation $\mathcal{I}$ of the functional $\mathcal{I}^{\mathrm{p}}$. Define $\mathcal{E} : [0, T] \times \mathcal{P} \times \mathcal{V} \to \mathbb{R}$ and $\mathcal{I} : [0, T] \times \mathcal{P} \to \mathbb{R}$ via

$$\mathcal{E}(t, c, u) = \int_\Omega \mathbb{W}(c(x), \nabla u(x))\,\mathrm{d}x - \langle G(t), u\rangle,$$
$$\mathcal{I}(t, c) = \min\{\,\mathcal{E}(t, c, u) \mid u \in \mathcal{V}\,\}. \tag{4.6}$$

From [LeR00], Ch. 4, the following result follows immediately by subsequent minimization with respect to the elastic deformation.

Theorem 4.4. *Assume that $W_{e_i}(\cdot)$ satisfies* (3.1) *and* (3.2). *Then, the relaxation $\mathcal{I}$ of $\mathcal{I}^{\mathrm{p}}$, as defined in* (4.1), *is given by* (4.6).

Furthermore, $\mathbb{W}(\cdot, \cdot) : P \times \mathbb{R}^{d\times d} \to \mathbb{R}$ is cross-quasiconvex in the sense of [LeR00], *which implies that $\mathbb{W}(\cdot, F) : P \to R$ is convex for fixed F and $\mathbb{W}(c, \cdot) : \mathbb{R}^{d\times d} \to \mathbb{R}$ is quasiconvex for fixed $c \in P$.*

Unfortunately, only a limited number of examples are known, where $\mathbb{W}$ can be computed explicitly. The first such case is the one-dimensional case. There we have the formula

$$\mathbb{W}(c, F) = \mathcal{L}\left(\sum_{j=1}^{n} c^{(j)} \mathcal{L} W_{e_j} \right)(F) \quad \text{with } c = (c^{(1)}, \dots, c^{(n)})^T,$$

where $\mathcal{L}$ is the Legendre-Fenchel transform with

$$(\mathcal{L}W)(\sigma) = \inf\{\,\sigma F - W(F) \mid F \in \mathbb{R}\,\}.$$

In the quadratic case with $W_{e_i}(F) = \frac{1}{\eta^{(i)}}(F-A^{(i)})^2+\beta^{(i)}$ and $\eta^{(i)} > 0$ this gives $\mathbb{W}(c, F) = (F-A\cdot c)^2/\eta\cdot c + \beta\cdot c$.

The second case where the mixture function can be calculated is that of linearized elasticity with identical elastic tensor $\mathbf{C} \in \mathrm{Lin}(\mathbb{R}^{d\times d}_{\mathrm{sym}}, \mathbb{R}^{d\times d}_{\mathrm{sym}})$ which is positive definite, i.e., there exists $\alpha > 0$ such that

$$\mathbf{C}E{:}E \stackrel{\text{def}}{=} \sum_{i,j=1}^{d} (\mathbf{C}E)_{ij}E_{ij} \geqq \alpha E{:}E \quad \text{for all } E \in \mathbb{R}^{d\times d}_{\mathrm{sym}}. \tag{4.7}$$

We continue to use the abbreviation $E = \frac{1}{2}(F+F^T)-I$ for the linearized strain tensor. With $\mathbf{C}$ and a direction $\omega \in \mathbb{R}^d$ we associate the so-called acoustic tensor $\mathbb{A}(\omega) \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ via

$$[\mathbb{A}(\omega)a]\cdot a = \tfrac{1}{4}[\mathbf{C}(a\otimes\omega+\omega\otimes a)]{:}(a\otimes\omega+\omega\otimes a) \quad \text{for } a \in \mathbb{R}^d.$$

Proposition 4.5. *Assume that* $\mathbf{C}$ *satisfies* (4.7) *and that* W_{e_i} *has the form* (4.4). *Then,*

$$\mathbb{W}(c, F) = \sum_{i=1}^{n} c^{(i)} W_{e_i}(F) + w_{\mathrm{mix}}(c), \tag{4.8}$$

where $w_{\mathrm{mix}} : P \to \mathbb{R}$ *is convex and satisfies* $w_{\mathrm{mix}}(e_j) = 0$ *and the bounds*

$$0 \geqq w_{\mathrm{mix}}(c) \geqq -\tfrac{1}{2}\sum_{j=1}^{n} c^{(j)}[\mathbf{C}A_j]{:}A_j + \tfrac{1}{2}\big[\mathbf{C}A^c\big]{:}A^c$$

with $A^c = \sum_{j=1}^{n} c^{(j)}A_j$. *Moreover, if* $A_j = A_0 + a^{(j)}A$ *for* $j = 1, \dots, n$, *then there is the explicit formula*

$$w_{\mathrm{mix}}(c) = -\frac{\gamma}{2}\Big[\sum_{j=1}^{n}\big(a^{(j)}\big)^2 c^{(j)} - (a\cdot c)^2\Big] \text{ with } a = (a^{(1)}, \dots, a^{(n)})$$
$$\text{and } \gamma = \max\left\{|\mathbb{A}(\omega)^{-1/2}(\mathbf{C}A)\omega|^2 \;\middle|\; |\omega| = 1\right\}. \tag{4.9}$$

In the case $n = 2$ the explicit formula (4.9) is always applicable. The first part of the assertion follows from the quadratic nature of the problem, see, e.g., [Kha67, Roi67, Kha83, Koh91] where also the case $n = 2$ was solved. Formula (4.9) for $n \geqq 3$ was established in [Mie00, GMH02] and applied to a particular PT problem with one austenite and two martensitic phases in [PAM98]. For partial results in more generals situations we also refer to [SmW98, Mie00].

Hence, we arrive at the following special case of Theorem 4.4.

Theorem 4.6. *Let* $\langle G(t), u\rangle = \int_\Omega g(t,x)\cdot u(t,x)\,\mathrm{d}x$ *and let* W_{e_j} *be given as in Proposition 4.5 and* $\mathcal{E}$ *and* $\mathcal{I}$ *as in* (4.6) *with* $\mathbb{W}$ *from* (4.8). *Then,*

$$\begin{aligned}\mathcal{I}(t,c) &= \min\left\{\,\mathcal{E}(t,c,u)\;\middle|\; u\in\mathcal{V}\subset \mathrm{W}^{1,2}(\Omega)\,\right\}\\ &= \eta(t)+\int_\Omega [(L_0c)(x)+\widehat{g}(t,x)]\cdot c(x)+w_{\mathrm{mix}}(c(x))\,\mathrm{d}x,\end{aligned}$$

where $L_0\in \mathrm{Lin}(Y,Y)$ *with* $Y=\mathrm{L}^2(\Omega,\mathbb{R}^n)$ *is a self-adjoint operator and* $\widehat{g}(t,\cdot)\in Y$.

Proof. The validity of Theorem 4.4 in this special case is also proved in [The01]. The second identity follows immediately from the first by using the quadratic nature and the fact that $\mathrm{L}^1(\Omega,P)$ can be embedded continuously into Y. Minimization in u does not involve w_{mix} and it follows that the minimizer $u=\mathcal{U}(G(t),c)$ depends linearly on $G(t)$ and c, i.e., $\mathcal{U}(G,c)=K_1G+K_2c$ with $K_1\in\mathrm{Lin}(\mathcal{V}^*,\mathcal{V})$ and $K_2\in\mathrm{Lin}(Y,\mathcal{V})$. Inserting this linear expression gives the desired quadratic expression. □

In Section 5 we will use this quadratic structure as well as the fact that L_0 is a pseudo-differential operator of order 0 whose symbol is positive definite.

4.3. Relaxation of the dissipation functional

The relaxation $\mathcal{D}:\mathcal{P}\times\mathcal{P}\to\mathbb{R}_{\geqq}$ of the function $\mathcal{D}^{\mathrm{p}}:\mathcal{P}^{\mathrm{p}}\times\mathcal{P}^{\mathrm{p}}\to\mathbb{R}_{\geqq}$ as defined in (4.2) can be calculated much easier, since $\mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}},c^{\mathrm{p}})$ depends on a^{p} and c^{p} only through a simple integration over the point values of $D^{\mathrm{p}}(a^{\mathrm{p}}(x),c^{\mathrm{p}}(x))$. For $(a,c)\in P\times P$ we set

$$D(a,c)=\inf\left\{\sum_{j,i=1}^n m_{ji}\kappa_{j\to i}\;\middle|\; m_{ji}\geqq 0,\ \sum_{i=1}^n m_{ji}=a^{(j)},\ \sum_{j=1}^n m_{ji}=c^{(i)}\right\}. \tag{4.10}$$

Clearly D is obtained by minimizing $D^{\mathrm{p}}(a^{\mathrm{p}},c^{\mathrm{p}})$ over $a^{\mathrm{p}},c^{\mathrm{p}}\in\mathrm{L}^1(B,P^{\mathrm{p}})$ under the constraints $a=⨍_B a^{\mathrm{p}}(y)\,\mathrm{d}y$ and $c=⨍_B c^{\mathrm{p}}(y)\,\mathrm{d}y$. The coefficients m_{ji} in (4.10) are simply the relative measures of the sets $\{\,y\in B\mid a(y)=e^{(j)},\ c(y)=e^{(i)}\,\}$. Using $\kappa_{j\to j}=0$, $\kappa_{\min}=\min\{\,\kappa_{j\to i}\mid j\neq i\,\}$, and $\kappa_{\max}=\max\{\,\kappa_{j\to i}\mid j\neq i\,\}$, we immediately find

$$\frac{\kappa_{\min}}{2}|c-a|_1\leqq D(a,c)\leqq\frac{\kappa_{\max}}{2}|c-a|_1\quad\text{where } |b|_1\overset{\mathrm{def}}{=}\sum_{j=1}^n|b^{(j)}|. \tag{4.11}$$

We also have $D(e_j,c)=\sum_{i=1}^n c^{(i)}\kappa_{j\to i}$. Since the difference $c-a$ for $a,c\in P$ will play a major role we define the linear space

$$\mathbb{R}^n_*=\{\,z\in\mathbb{R}^n\mid z\cdot e_*=0\,\}\quad\text{where } e_*=(1,\dots,1)^T.$$

Proposition 4.7. *The function $D : P \times P \to [0, \infty)$ is convex, i.e.,*

$$D(\theta a_1+(1-\theta)a_2, \theta c_1+(1-\theta)c_2) \leqq \theta D(a_1, c_1) + (1-\theta)D(a_2, c_2) \quad \text{for } \theta \in [0, 1].$$

If D^{p} satisfies the triangle inequality (3.4)*, then so does D and there exists a unique function $\Delta : \mathbb{R}^n_* \to [0, \infty)$ which is homogeneous of degree* 1 *(i.e., $\Delta(\alpha b) = \alpha\Delta(b)$ for $\alpha \geqq 0$ and $b \in \mathbb{R}^n_*$) such that D has the form*

$$D(a, c) = \Delta(c-a) \quad \text{for all } a, c \in P. \tag{4.12}$$

Remark 4.8. The triangle inequality plays a twofold role. First, it guarantees the difference representation with Δ. Second, it guarantees the stability of the solutions of the incremental problem. To illustrate the necessity in both cases, consider a situation with three phases. Let $\kappa_{1\to 3} = \kappa$ and $\kappa_{j\to i} = 1$ else for $i \neq j$. For the volume fractions $a = (1/4, \alpha, 3/4-\alpha)^T$ and $c = (0, \alpha, 1-\alpha)^T$, we have $c-a = (-1/4, 0, 1/4)^T$ which is independent of α. For $\kappa \in (0, 2]$ the triangle inequality holds and we find $D(a, c) = \kappa/4$. For $\kappa > 2$ and $\alpha \in [0, 1/4]$ we have $D(a, c) = 2\alpha+(1-4\alpha)\kappa/4$ which clearly contradicts the difference formula.

Moreover, consider the trivial energies $\mathcal{I}^{\mathrm{p}}(t, e_j) = 6-2j$ together with the initial state $c^{\mathrm{p}}_0 = e_1$. Then, $\mathcal{I}^{\mathrm{p}}(t, c^{\mathrm{p}}) + D^{\mathrm{p}}(e_1, c^{\mathrm{p}})$ is minimized with $c^{\mathrm{p}} = e_2$ for $\kappa \geqq 3$ and with $c^{\mathrm{p}} = e_3$ for $\kappa \leqq 3$. However, e_2 is never stable whereas e_3 is always stable.

Proof. Consider $a_i, c_i \in P$ and let $m^{(i)}_{jk}$ be the minimizers in the definition of $D(a_i, c_i)$ for $i = 1, 2$, that is $m^{(i)}_{jk} \geqq 0$, $\sum_{l=1}^n m^{(i)}_{jl} = a^{(j)}_i$, and $\sum_{j=1}^n m^{(i)}_{jl} = c^{(l)}_i$. Then, $m^{(3)}_{jl} = \theta m^{(1)}_{jl} + (1-\theta)m^{(2)}_{jl}$ forms an admissible set in the definition of $D(\theta a_1+(1-\theta)a_2, \theta c_1+(1-\theta)c_2)$, which gives the convexity result after separating the minimum into the weighted sum of two minima. The triangle inequality for D follows by a straightforward use of its definition and (3.4).

The proof of the representation (4.12) involves the standard duality theory for linear transport problems as developed in the textbooks [Gal60, Gas58]. This theory implies the dual representation

$$D(a, c) = \max\left\{ \mu \cdot c - \nu \cdot a \mid \mu, \nu \in \mathbb{R}^n \text{ with } \mu^{(j)}-\nu^{(i)} \leqq \kappa_{i\to j} \text{ for all } i, j \right\}.$$

Using the triangle inequality, we now have to show that in the above maximum we can restrict the variables μ and ν to the case $\mu = \nu$, which then gives the function

$$\Delta(c-a) \stackrel{\text{def}}{=} \max\left\{ \mu \cdot (c-a) \mid \mu \in \mathbb{R}^n,\ \mu^{(j)}-\mu^{(i)} \leqq \kappa_{i\to j} \text{ for } i, j \right\}. \tag{4.13}$$

To this end we employ the following standard optimality condition. If (m_{ij}) is a minimizer in (4.10) and (μ, ν) a maximizer in the dual formulation then

$$m_{ij} > 0 \quad \text{implies} \quad \kappa_{i\to j} = \mu^{(j)}-\nu^{(i)}. \tag{4.14}$$

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

Using the triangle inequality we show that it is always possible to find a minimizer (m_{ij}) in (4.10) which satisfies

$$m_{ii} = \sigma_i \quad \text{with } \sigma_i \stackrel{\text{def}}{=} \min\{a^{(i)}, c^{(i)}\} \text{ for } i = 1, \dots, n. \tag{4.15}$$

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

Using identity (4.15) and the extremality condition (4.14) we conclude that $\mu = \nu$ in the dual problem whenever a and c have positive coordinates. Then, the desired relation $D(a, c) = \Delta(c-a)$ follows. By continuity of D and Δ it immediately extends to all of $P \times P$. □

We now define the integrated function $\mathbf{\Delta} : \mathrm{L}^1(\Omega, \mathbb{R}^n_*) \to \mathbb{R}_{\geqq}$ via

$$\mathbf{\Delta}(z) = \int_\Omega \Delta(z(x))\,\mathrm{d}x. \tag{4.16}$$

Under the assumption that D^{p} satisfies the triangle inequality we have $D^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}}) = \Delta(c^{\mathrm{p}} - a^{\mathrm{p}})$ and hence $\mathcal{D}^{\mathrm{p}}(a^{\mathrm{p}}, c^{\mathrm{p}}) = \mathbf{\Delta}(c^{\mathrm{p}} - a^{\mathrm{p}})$ for all $a^{\mathrm{p}}, c^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$.

Theorem 4.9. *Assume that $D^{\mathrm{p}} : P^{\mathrm{p}} \times P^{\mathrm{p}} \to \mathbb{R}_{\geqq}$ satisfies the triangle inequality* (3.4). *Then, the relaxation $\mathcal{D} : \mathcal{P} \times \mathcal{P} \to \mathbb{R}_{\geqq}$ defined in* (4.2) *is given by $\mathcal{D}(a, c) = \mathbf{\Delta}(c-a)$. It satisfies the triangle inequality and $\kappa_{\min}\|c-a\|_{\mathrm{L}^1} \leqq 2\mathcal{D}(a, c) \leqq \kappa_{\max}\|c-a\|_{\mathrm{L}^1}$.*

The proof can be found in [The01].

4.4. The separately relaxed incremental problem

Using these two relaxed functionals we obtain a relaxed formulation of the incremental problem (IP). With $\mathcal{I}$ from (4.6) and $\mathbf{\Delta}$ from (4.16) we postulate the following *separately relaxed incremental problem*:

(SRIP) For given $c_0 \in \mathcal{P}$, find $c_1, \dots, c_N \in \mathcal{P}$ such that

$$\mathcal{I}(t_k, c_k) + \mathbf{\Delta}(c_k - c_{k-1}) = \inf\{\mathcal{I}(t_k, c) + \mathbf{\Delta}(c - c_{k-1}) \mid c \in \mathcal{P}\}$$

for $k = 1, \dots, N$.

Clearly, solutions $(c_k)_{k=1,\dots,N}$ of (SRIP) are stable and satisfy the incremental energy inequality (cf. Theorem 2.6), viz.,

$$\text{(S)} \quad \mathcal{I}(t_k, c_k) \leqq \mathcal{I}(t_k, a) + \mathbf{\Delta}(a - c_k) \quad \text{for all } a \in \mathcal{P},$$

$$\text{(E)}_{\text{incr}} \quad \mathcal{I}(t_k, c_k) + \mathbf{\Delta}(c_k - c_{k-1}) \leqq \mathcal{I}(t_k, c_{k-1}) = \mathcal{I}(t_{k-1}, c_{k-1}) + \int_{t_{k-1}}^{t_k} \partial_t \mathcal{I}(s, c_{k-1})\,\mathrm{d}s.$$

There are two ways to see that (SRIP) always has a solution. In the first case we use the general construction of $\mathcal{I}$ and $\mathbf{\Delta}$ which implies that $\mathcal{J}_k(a,\cdot) : \mathcal{P} \to \mathbb{R}$; $c \mapsto \mathcal{I}(t_k, c) + \mathbf{\Delta}(c-a)$ is weakly lower semicontinuous. Since $\mathcal{P}$ is bounded in $\mathrm{L}^\infty(\Omega, \mathbb{R}^d)$ the existence of a minimizer follows. The second approach to the existence of minimizers $c \in \mathcal{P}$ is much more useful for doing actual numerics. We reintroduce $u \in \mathcal{V}$ and minimize the functional

$$\begin{aligned}\mathcal{G}_k(a,c,u) &= \mathcal{E}(t_k,c,u) + \mathbf{\Delta}(c-a)\\ &= \int_\Omega \mathbb{W}(c(x), \nabla u(x)) + \Delta(c(x)-a(x))\,\mathrm{d}x - \langle G(t), u\rangle\end{aligned}$$

with respect to $(c,u) \in \mathcal{P}\times\mathcal{V}$. As $c(x)$ appears only locally in the integral we may minimize with respect to c first and do the minimization pointwise in $x \in \Omega$. For this purpose define the *reduced incremental energy density*

$$\Psi^{\mathrm{red}}(a,F) = \min\{\,\mathbb{W}(c,F) + \Delta(c-a) \mid c \in P\,\}, \tag{4.17}$$

where, by continuity of $\mathbb{W}(\cdot,F) + \Delta(\cdot - a)$, the minimum is achieved at $c = C(a,F)$, i.e., $\Psi^{\mathrm{red}}(a,F) = \mathbb{W}(C(a,F),F) + \Delta(C(a,F)-a)$. The cross-quasiconvexity of $\mathbb{W}$ implies that, for each $a \in P$, the function $\Psi^{\mathrm{red}}(a,\cdot)$ is quasiconvex, cf. [LeR00]. Hence, the functional

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

is weakly lower semicontinuous, cf. the general theory in [Dac89, FKP94, LeR00]. For our special case of Proposition 4.5 with $n = 2$ the functions Ψ^{red} and C can be given explicitly, see [MTL98, MiT99, CaP00]. Now, (SRIP) can be reformulated as follows.

(SRIP)′ For $c_0^{\mathrm{p}} \in \mathcal{P}^{\mathrm{p}}$, find $(c_1,u_1),\dots,(c_N,u_N) \in \mathcal{P}\times\mathcal{V}$ such that

$$\mathcal{G}^{\mathrm{red}}(t_k, c_{k-1}, u_k) = \inf\{\,\mathcal{G}^{\mathrm{red}}(t_k, c_{k-1}, v) \mid v \in \mathcal{V}\,\}$$

and then let $c_k(x) = C(c_{k-1}(x), \nabla u_k(x))$.

The formulation of (SRIP)′ has the major advantage that it reduces to a simple variational problem for the variable $u_k \in \mathcal{V}$. By the quasiconvexity of $\Psi^{\mathrm{red}}(a,\cdot)$ the existence of a minimizer is clear. The important message is that the function Ψ^{red} 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 (SRIP). (Similar reduced densities and functionals appear in elasto-plasticity [CHM02, Mi02a].)

4.5. The relaxed time-continuous problem

One reason for choosing the separate relaxation was to obtain rather explicit results. The second reason is that the structure of the problem remains the same. In particular, (SRIP) can be interpreted as the incremental version of a new time-continuous relaxed problem. The functionals $\mathcal{I}$ and $\mathbf{\Delta}$ constructed above are now the ones used in the abstract existence theory of Section 2. The *separately relaxed time-continuous problem* is exactly that of the existence of an admissible process as stated in the abstract section.

(SRCP) Given $c_0 \in \mathcal{P}$, find $c : [0, T] \to \mathcal{P}$ with $c(0) = c_0$ such that $c(t) \in \mathcal{P}$ is stable for all $t \in (0, T]$ and that the weak energy inequality holds, viz.,

(S) $\mathcal{I}(t, c(t)) \leqq \mathcal{I}(t, a) + \mathbf{\Delta}(a - c(t))$ for all $t \in (0, T]$ and $a \in \mathcal{P}$,

(E) $\mathcal{I}(T, c(T)) + \displaystyle\int_0^T \Delta(\mathrm{d}c) \leqq \mathcal{I}(0, c_0) - \int_0^T \langle \dot{G}(t), u(t) \rangle \, \mathrm{d}t$,

where $u(t) = \mathcal{U}(G(t), c(t))$ is a minimizer of $\mathcal{E}(t, c(t), \cdot)$.

Note that in our situation we have $\partial_t \mathcal{I}(t, c) = -\langle \dot{G}(t), \mathcal{U}(G(t), c(t)) \rangle$ such that we are in accordance with (E).

According to Section 2.3 we can associate with (SRCP) an incremental problem to obtain solutions. By construction this is exactly the separately relaxed incremental problem (SRIP) we started with. It is the purpose of the next section to show that the assumptions of the abstract existence theory are satisfied for a nontrivial special case. Thus, we are able to conclude that there exist solutions for (SRCP).

Remark 4.10. The above relaxation can be understood as a Young-measure relaxation as studied in [Mi02b]. The space $\mathrm{L}^1(\Omega, P)$ is exactly $\mathrm{YM}(\Omega, P^{\mathrm{p}})$, the set of Young measures on Ω taking values in $\mathrm{Prob}(P^{\mathrm{p}})$ where $\mathrm{Prob}(P^{\mathrm{p}})$ is identified with $P = \mathrm{conv}(P^{\mathrm{p}})$. Note that P^{p} is finite and P compact. By construction, the distance $D : P \times P \to [0, \infty)$ is exactly the Wasserstein distance on $\mathrm{Prob}(P^{\mathrm{p}})$ associated with the distance $D^{\mathrm{p}} : P^{\mathrm{p}} \times P^{\mathrm{p}} \to [0, \infty)$ on P^{p}.

Finally we show that (SRCP) can be interpreted as a doubly nonlinear differential inclusion which looks similar to flow rules in plasticity, cf. [CoV90, MiT02, Mi02a]. This will be a specification of the abstract flow rules discussed in Theorem 2.3. In the engineering literature such flow rules are used for phase transformation problems as well, see [HaG99, GMH02].

Here we use specifically that $\mathcal{P} = \mathrm{L}^1(\Omega, P)$ and $\mathbf{\Delta}(z) = \int_\Omega \Delta(z(x)) \, \mathrm{d}x$ are given pointwise in $x \in \Omega$. This allows us to make the differential inclusion (2.9) quite explicit. Define $\Sigma \subset \mathbb{R}^n_* = \{ z \in \mathbb{R}^n \mid z \cdot e_* = 0 \}$ via the subdifferential of $\Delta : \mathbb{R}^n_* \to \mathbb{R}$ as $\Sigma = \partial \Delta(0)$. According to (4.13) we have

$$\Sigma = \mathrm{conv}\{\sigma_1, \dots, \sigma_N\} \quad \text{and} \quad \Delta(z) = \max \left\{ z \cdot \sigma_j \mid j = 1, \dots, N \right\}.$$

In particular we find $\mathbf{\Sigma} = \left\{ \sigma \in \mathrm{L}^\infty(\Omega, \mathbb{R}^n_*) \mid \sigma(x) \in \Sigma \text{ for a.e. } x \in \Omega \right\}$ and

$$\partial \mathbf{\Delta}(z) = \{ \sigma \in \mathbf{\Sigma} \mid \sigma(x) \cdot z(x) = \Delta(z(x)) \text{ for a.e. } x \in \Omega \}.$$

Similarly the outer normal cone $\partial\mathcal{X}_{\mathcal{P}}(c) = \mathrm{N}_c\mathcal{P}$ can be characterized pointwise

$$\mathrm{N}_c\mathcal{P} = \left\{ \sigma \in \mathrm{L}^\infty(\Omega, \mathbb{R}^n_*) \mid \sigma(x) \in \mathrm{N}_{c(x)}P \text{ for a.e. } x \in \Omega \right\},$$

where $\mathrm{N}_{c(x)}P \subset \mathbb{R}^n_*$ is the finite-dimensional normal cone of the polytope P.

The derivative of the functional $\mathcal{I}(t,\cdot)$ is best represented by reintroducing the deformation u and the associated equation for the elastic equilibrium. Recall for this end that $\mathcal{I}(t,c)$ was defined by minimizing $\mathcal{E}(t,c,u)$ with respect to $u \in \mathcal{V}$. This leads to the doubly nonlinear form ([CoV90, MiT02]) of the problem:

$$\begin{aligned} 0 &= \mathrm{D}_u\mathcal{E}(t, c(t), u(t)),\\ 0 &\in \partial\boldsymbol{\Delta}(\dot{c}(t)) + \mathrm{D}_c\mathcal{E}(t, c(t), u(t)) + \mathrm{N}_{c(t)}\mathcal{P}. \end{aligned}$$

Here the first equation is the classical elliptic system describing the elastic equilibrium and the second relation is a flow rule for $c(t,x)$ which is completely local in $x \in \Omega$. With $\langle G(t), u\rangle = \int_\Omega g(t,x)\cdot u(t,x)\,\mathrm{d}x$, the full problem can be written as follows.

Local flow formulation. For almost all $(t,x) \in [0,T]\times\Omega$ we have

$$\begin{aligned} 0 &= \mathrm{div}_x \frac{\partial}{\partial F}\mathbb{W}(x, \nabla_x u(t,x), c(t,x)) + g(t,x)\\ 0 &\in \partial\Delta(\dot{c}(t,x)) + \frac{\partial}{\partial c}\mathbb{W}(\nabla_x u(t,x), c(t,x)) + \mathrm{N}_{c(t,x)}P. \end{aligned} \tag{4.18}$$

together with the standard boundary conditions.

The second relation can be reformulated without the subdifferential of Δ:

$$\begin{aligned} &\exists\, n(t,x) \in \mathrm{N}_{c(t,x)}P \text{ such that}\\ &\Delta(\dot{c}(t,x)) + \dot{c}(t,x)\cdot\left[\frac{\partial}{\partial c}\mathbb{W}(\nabla_x u(t,x), c(t,x)) + n(t,x)\right] = 0 \end{aligned}$$

for a.e. $(t,x) \in [0,T]\times\Omega$. Recall that $\mathbb{W}$ is convex in $c \in P$, however it may not be differentiable. In such a case we may replace the partial derivative $\frac{\partial}{\partial c}\mathbb{W}(F,c)$ by any element in the subdifferential $\partial_c\mathbb{W}(F,c)$.

5. Existence of admissible processes for a special case

We now restrict our view completely to the case of linearized elasticity with two phases (n=2) whose elastic tensors are identical. For this case the mixture function $\mathbb{W}$ is given explicitly in Proposition 4.5. We simplify the notation by identification of $P = \mathrm{conv}\{e_1, e_2\} \subset \mathbb{R}^2$ with the interval $[0,1]$ via the mapping $[0,1] \ni \theta \mapsto (1-\theta)e_1 + \theta e_2$. Moreover, we will use the (infinitesimal) displacement $\widetilde{u} : \Omega \to \mathbb{R}^d$ rather than the displacement $u : x \mapsto x + \varepsilon\widetilde{u}(x)$, where ε is a small parameter. We will consider phase distributions $\theta \in \mathcal{P} = \mathrm{L}^1(\Omega,[0,1]) \subset X \stackrel{\mathrm{def}}{=} \mathrm{L}^1(\Omega,\mathbb{R})$ and displacements $\widetilde{u} \in \mathcal{V} = \left\{ v \in \mathrm{W}^{1,2}(\Omega,\mathbb{R}^d) \mid v|_\Gamma = 0 \right\}$, where Γ is that part of $\partial\Omega$ where Dirichlet boundary conditions are prescribed.

The mixture function takes the specific form

$$\mathbb{W}(\theta, E) = \tfrac{1-\theta}{2}\mathbf{C}[E-A_1]:(E-A_1)+\tfrac{\theta}{2}\mathbf{C}[E-A_2]:(E-A_2)-\tfrac{\gamma}{2}\theta(1-\theta), \quad (5.1)$$

where $\mathbf{C}$ satisfies (4.7) and γ is defined in (4.9) with $A = A_2-A_1$. The dissipation functional now reads $\mathbf{\Delta} : X \to \mathbb{R}_{\geqq}; \zeta \mapsto \int_\Omega \Delta(\zeta(x))\,\mathrm{d}x$ with $\kappa_{1\to 2}, \kappa_{2\to 1} > 0$ and

$$\Delta : \mathbb{R} \to \mathbb{R}_{\geqq}; \zeta \mapsto \max\{\zeta\kappa_{1\to 2}, -\zeta\kappa_{2\to 1}\}. \quad (5.2)$$

The aim of this section is to proof an existence theorem for the separately relaxed problem (SRCP) for this special case. The following result gives a typical situation. However, slight generalizations are possible.

Theorem 5.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with C^1 boundary and $\mathcal{P}$, X, $\mathcal{V}$, $\mathbf{\Delta}$, and $\mathbb{W}$ as above. Moreover, assume $G \in \mathrm{C}^1([0,T], \mathcal{V}^*)$ and let*

$$\mathcal{I}(t,\theta) = \min\left\{ \int_\Omega \mathbb{W}(\theta, \frac{1}{2}(\nabla\widetilde{u}+\nabla\widetilde{u}^T))\,\mathrm{d}x + \langle G(t), \widetilde{u}\rangle \;\middle|\; \widetilde{u} \in \mathcal{V}\right\}.$$

If additionally either (a) *or* (b) *hold, where*

(a) $\Gamma = \partial\Omega$ (*full Dirichlet conditions*),
(b) $A_2-A_1 = b\otimes\xi+\xi\otimes b$ *for some* $b, \xi \in \mathbb{R}^d$ (*infinitesimally rank-one connected wells*),

then for each $c_0 \in \mathcal{P}$ there exists an admissible process in the sense of Definition 2.1, i.e., a solution of (SRCP).

The proof of this result constitutes the remainder of this section. In fact, we can strengthen the result slightly. If (a) as well as certain algebraic conditions on $\mathbf{C}$ and A_2-A_1 hold, it is possible to prove strict convexity of $\mathcal{I}(t,\cdot)$, see Remark 5.6 at the end of this section. Then, Theorem 7.5 in [MiT02] implies continuity of $c : (0,T] \to \mathcal{P}$.

Our special case can be handled due to the fact that $\mathbb{W}$ is quadratic in c and ∇u. Hence, it is possible to work out the form of $\mathcal{I}(t,\theta)$ more explicitly than in Theorem 4.6. We use also the Hilbert space $Y = \mathrm{L}^2(\Omega, \mathbb{R})$, which is possible since the weak and strong topologies on $\mathcal{P}$ which are induced by Y and X are the same.

Proposition 5.2. *If the assumptions of Theorem 5.1* (*but not necessarily* (a) *or* (b)) *hold, then there exist $\eta \in \mathrm{C}^1([0,T], \mathbb{R})$, $\widehat{g} \in \mathrm{C}^1([0,T], Y)$ and a symmetric operator $L \in \mathrm{Lin}(Y, Y)$ such that*

$$\mathcal{I}(t,\theta) = \eta(t) + \int_\Omega \left[(\tfrac{1}{2}L\theta)(x) + \widehat{g}(t,x)\right]\theta(x)\,\mathrm{d}x.$$

Moreover, L is a pseudo-differential operator of order 0 which has the symbol $\ell : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$ given by

$$\ell(\omega) = \gamma - \lambda(\omega) \text{ with } \lambda(\omega) = \left[\mathbb{A}(\omega)^{-1}(\mathbf{C}A)\omega\right]\cdot[(\mathbf{C}A)\omega], \quad (5.3)$$

where $A = A_2-A_1$, and hence is nonnegative, cf. (4.9).

Proof. We have to minimize $\mathcal{E}(t,\theta,\widetilde{u})$, which is quadratic in $(\theta,\widetilde{u}) \in Y \times \mathcal{V}$ with respect to $\widetilde{u} \in \mathcal{V}$. We obtain the unique minimizer $\widetilde{u} = K_1 G(t) + K_2\theta$ where $K_1 \in \mathrm{Lin}(\mathcal{V}^*, \mathcal{V})$ and $K_2 \in \mathrm{Lin}(Y, \mathcal{V})$. Note that K_2 is a pseudo-differential operator of order -1. Inserting this result into $\mathcal{E}(t,\cdot)$ defines the differentiable functions $t \mapsto \eta(t) \in \mathbb{R}$ and $t \mapsto \widehat{g}(t) \in Y$ and the pseudo-differential operator L of order 0, as $E = \frac{1}{2}(\nabla\widetilde{u}+\nabla\widetilde{u}^T)$ is a differential operator of order 1.

It remains to calculate the symbol of L. This is done most easily by inserting $E = E_{a,\omega} \stackrel{\text{def}}{=} \frac{1}{2}(a\otimes\omega + \omega\otimes a) \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ into the quadratic part of $\mathbb{W}$ which gives

$$\tfrac{1}{2}\mathbf{C}E_{a,\omega}{:}E_{a,\omega} - \theta\mathbf{C}E_{a,\omega}{:}A + \theta^2\tfrac{\gamma}{2} = \tfrac{1}{2}\mathbb{A}(\omega)a\cdot a - \theta\mathbf{C}A\omega\cdot a + \theta^2\tfrac{\gamma}{2}.$$

A subsequent minimization with respect to $a \in \mathbb{R}^d$ yields the desired result. □

From the theory of pseudo-differential operators, it follows that the range of the symbol ℓ constitutes the continuous spectrum whereas compact perturbations which are not seen in the symbol may generate additional discrete eigenvalues. Such compact perturbations arise from the different boundary conditions for the displacement $\widetilde{u}$. However, we conclude that the (strictly) negative part of L must be compact and it is exactly this property which guarantees weak lower semicontinuity of $\mathcal{I}(t,\cdot) : Y \to \mathbb{R}$ and hence that of $\mathcal{I}(t,\cdot) : \mathcal{P} \subset \mathrm{L}^1(\Omega,\mathbb{R}) \to \mathbb{R}$. It is remarkable that the continuous spectrum always includes 0, as the definition of γ is just such that the minimum of $\ell(\omega)$, $0 \neq \omega \in \mathbb{R}^d$ is 0. This implies that $\mathcal{I}$ can never be uniformly convex. However, strict convexity is still possible depending on the compact perturbations through the boundary conditions.

Our subsequent existence result will work for all cases where L is positive semi-definite. Thus, we give some cases where this can be guaranteed. We now have to take into account the boundary conditions for $\widetilde{u}$. We recall that $\Gamma \subset \partial\Omega$ is that part of the boundary where we have imposed Dirichlet data, i.e., $\widetilde{u}|_\Gamma = 0$.

Lemma 5.3. *The operator L is positive semi-definite if either* (a) *or* (b) *in Theorem 5.1 holds.*

Proof. The idea of the proof is to return to the quadratic functional $\mathcal{E}(t,\theta,\widetilde{u})$ and to eliminate θ first, cf. Section 4.4 and the derivation of (SRIP)′ for the analogous strategy. Consider the quadratic form

$$Q(\theta,\widetilde{u}) = \int_\Omega \frac{1}{2}\mathbf{C}E(\widetilde{u}){:}E(\widetilde{u}) - \theta\mathbf{C}E(\widetilde{u}){:}A + \theta^2\frac{\gamma}{2}\,\mathrm{d}x,$$

with $E(\widetilde{u}) = \frac{1}{2}(\nabla\widetilde{u}+\nabla\widetilde{u}^T)$, which is the homogeneous part of degree 2 of $\mathcal{E}$.

On the one hand we have $\int_\Omega (L\theta)\theta\,\mathrm{d}x = 2\min\{\,Q(\theta,\widetilde{u}) \mid u \in \mathcal{V}\,\}$. On the other hand we may eliminate θ first to obtain

$$\widehat{Q}(\widetilde{u}) = \min\{\,Q(\theta,\widetilde{u}) \mid \theta \in Y\,\} = \int_\Omega \frac{1}{2}\widehat{\mathbf{C}}E(\widetilde{u}){:}E(\widetilde{u})\,\mathrm{d}x,$$

where the reduced elasticity tensor $\widehat{\mathbf{C}}$ is given by $\widehat{\mathbf{C}}E{:}E = \mathbf{C}E{:}E - [\mathbf{C}E{:}A]^2/\gamma$. Clearly we have $L \geqq 0$ if and only if $\widehat{Q}(u) \geqq 0$ for all $u \in \mathcal{V}$. Since $\widehat{Q}$ is homogeneous, the last condition is equivalent to convexity of $\widehat{Q}$.

The case (a) is now obtained by studying the symbol associated with $\widehat{Q}$ which takes the form $S(\omega) = \mathbb{A}(\omega) - \frac{1}{\gamma}[(\mathbf{C}A)\omega]\otimes[(\mathbf{C}A)\omega]$. Using $a = \mathbb{A}(\omega)^{-1/2}b$ we find

$$S(\omega)a\cdot a = |b|^2 - \tfrac{1}{\gamma}[(\mathbf{C}A)\omega\cdot\mathbb{A}(\omega)^{-1/2}b]^2 \geqq |b|^2\Big(1-\tfrac{1}{\gamma}|\mathbb{A}(\omega)^{-1/2}(\mathbf{C}A)\omega|^2\Big),$$

and using the definition of γ shows that the symbol is always positive semi-definite. This means that the function $F \mapsto \frac{1}{4}\widehat{\mathbf{C}}(F+F^T):(F+F^T)$ is rank-one convex. Together with the full Dirichlet condition this implies convexity of $\widehat{Q}$, cf. [Dac89].

For the case (b) we cannot use the boundary conditions. Instead we show convexity of $\widehat{Q}$ by convexity of the integrand, i.e., $\widehat{\mathbf{C}}E:E \geqq 0$ for all $E \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$. We define a scalar product on $\mathbb{R}^{d\times d}_{\mathrm{sym}}$ via $\langle\langle E_1, E_2\rangle\rangle = \mathbf{C}E_1:E_2$. Then, on the one hand we have $\widehat{\mathbf{C}}E:E = \langle\langle E, E\rangle\rangle - \langle\langle E, A\rangle\rangle^2/\gamma$; and convexity holds, by the Cauchy-Schwarz inequality, if and only if $\langle\langle A, A\rangle\rangle \leqq \gamma$. On the other hand γ takes the form

$$\gamma = \max\Big\{\, \langle\langle E_{a,\omega}, A\rangle\rangle^2/\langle\langle E_{a,\omega}, E_{a,\omega}\rangle\rangle \;\mid\; 0 \neq a, \omega \in \mathbb{R}^d \,\Big\} \leqq \langle\langle A, A\rangle\rangle.$$

By assumption (b), $A = E_{b,\xi}$ is an admissible candidate in the maximum and we conclude that $\gamma = \langle\langle A, A\rangle\rangle$ and, hence, the desired convexity follows. □

We now want to apply the abstract theory of Section 2. Clearly, the quadratic form of $\mathcal{I}$ and the continuous differentiability in t implies that all necessary continuity assumptions are satisfied for $\mathcal{I}$ and $\mathbf{\Delta}$. Thus, Theorem 2.6 is applicable and we have solutions of the incremental problem (SRIP) which are stable and satisfy the discrete energy inequality. The compactness condition (2.11) for $\mathcal{P} \subset Y \subset X$ is also fulfilled and thus Corollary 2.8 allows us to extract a limit function θ^∞ such that $\theta = (\theta^\infty)^-$ is a suitable candidate for the solution of (SRCP). The abstract existence theorem, Theorem 2.9, has two further assumptions. The first is the weak continuity of the mapping $\theta \mapsto \partial_t\mathcal{I}(t,\cdot)$ which clearly holds due to linearity.

The second condition is the weak closedness of the set of stable states

$$\mathcal{S}(t) = \big\{\, \theta \in \mathcal{P} \;\mid\; \mathcal{I}(t,\theta) \leqq \mathcal{I}(t,\zeta) + \mathbf{\Delta}(\zeta-\theta) \text{ for all } \zeta \in \mathcal{P} \,\big\}.$$

It is here that we need to restrict our analysis to the case where L is positive semi-definite. We do not believe that this condition is really needed, but we were unable to find a proof for the more general case. Recall that convexity of $\mathcal{I}(t,\cdot)$ does not imply convexity of $\mathcal{S}(t)$; we have to use the theory of pseudo-differential operators in the form of the H-measure, also called microlocal defect measure [Tar90, Ger91].

Proposition 5.4. *If, in addition to the above assumptions, $L \geqq 0$, then the set of stable states $\mathcal{S}(t)$ is weakly closed for all $t \in [0,T]$.*

Proof. For simplicity we omit the dependence on t throughout the proof.

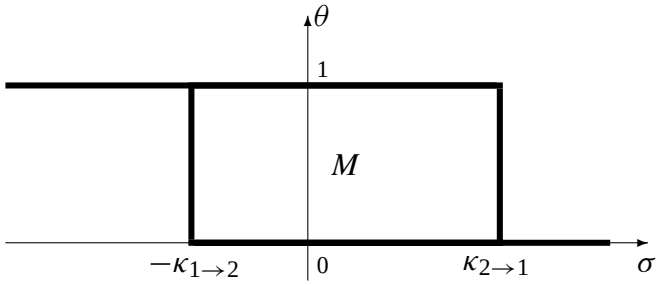

Fig. 5.1. The (nonconvex) set $M \subset \mathbb{R}^2$ is the filled rectangle plus the two infinite halflines

Clearly, $\mathcal{I}(t,\cdot) : Y \to \mathbb{R}$ is differentiable and convex due to $L \geqq 0$. Hence, $\theta \in \mathcal{S}$ if and only if $\mathrm{D}\mathcal{I}(\theta)[\zeta-\theta] + \mathbf{\Delta}(\zeta-\theta) \geqq 0$ for all $\zeta \in \mathcal{P}$. (In the nonconvex case this is necessary but not sufficient.) Written as integrals this gives

$$\int_\Omega [L\theta(x)+\widehat{g}(x)](\zeta(x)-\theta(x))+\Delta(\zeta(x)-\theta(x))\,\mathrm{d}x \geqq 0 \tag{5.4}$$

for $\zeta \in \mathcal{P} = \mathrm{L}^1(\Omega,[0,1])$. This condition has the big advantage that the test function ζ appears only locally under the integral. Thus, we can vary ζ pointwise and find that $\theta \in \mathcal{S}$ if and only if

$$(\theta(x), (L\theta)(x) + \widehat{g}(x)) \in M \quad \text{for a.e. } x \in \Omega, \tag{5.5}$$

where $M \subset \mathbb{R}^2$ is defined via

$$M = \left\{ (\theta,\sigma) \in [0,1] \times \mathbb{R} \mid (\sigma-\kappa_{2\to1})\theta \leqq 0,\ (\sigma+\kappa_{1\to2})(\theta-1) \leqq 0 \right\},$$

see Fig. 5.1. Note that M is not convex; however, roughly speaking, the proof works since intersections of M with lines of the form $(\theta, \ell\theta + \widehat{g})$ with $\ell \geqq 0$ are convex.

Now consider a sequence $\theta_k \in \mathcal{S} \subset \mathcal{P}$ which satisfies $\theta_k \rightharpoonup \theta_*$ in $Y = \mathrm{L}^2(\Omega)$. Clearly we then have $L\theta_k+\widehat{g} \rightharpoonup L\theta_*+\widehat{g}$. The following lemma shows the implication

$$\theta_k(L\theta_k) \rightharpoonup w \text{ in } X = \mathrm{L}^1(\Omega) \implies \theta_*(x)(L\theta_*)(x) \leqq w(x) \text{ a.e. in } \Omega. \tag{5.6}$$

Convexity just implies the weaker statement $\int_\Omega w\,\mathrm{d}x \geqq \int_\Omega \theta_*(L\theta_*)\,\mathrm{d}x$. Thus, we are able to control the sign of the quadratic expressions which appear in the definition of M. By (5.5) we know that $\theta_k \in \mathcal{S}$ is equivalent to

$$\begin{aligned}
&\theta_k(x) \in [0,1], \quad \theta_k(x)(L\theta_k)(x) \leqq (\widehat{g}(x)+\kappa_{2\to1})\theta_k(x),\\
&\theta_k(x)(L\theta_k)(x) \leqq (\widehat{g}(x)-\kappa_{1\to2})(\theta_k(x)-1) + (L\theta_k)(x) \text{ for a.e. } x \in \Omega.
\end{aligned}$$

Choosing a subsequence (k_l) such $\theta_{k_l}(L\theta_{k_l})$ converges to w weakly in X, we find for the limit θ_*, the estimates

$$\begin{aligned}
&\theta_*(x) \in [0,1], \quad w(x) \leqq (\widehat{g}(x)+\kappa_{2\to1})\theta_*(x),\\
&w(x) \leqq (\widehat{g}(x)-\kappa_{1\to2})(\theta_*(x)-1) + (L\theta_*)(x) \text{ for a.e. } x \in \Omega.
\end{aligned}$$

Together with $\theta_*(L\theta_*) \leqq w$ this implies $\theta_* \in \mathcal{S}$. □

Theorem 5.1 is established if the implication (5.6) is proved, which is the content of the following lemma.

Lemma 5.5. *Let L be a scalar pseudo-differential operator of order 0 with non-negative symbol ℓ. Assume that for $k \to \infty$ we have $\theta_k \rightharpoonup \theta_*$ in $\mathrm{L}^p(\Omega)$ and $\theta_k(L\theta_k) \rightharpoonup w$ in $\mathrm{L}^{p/2}(\Omega)$, where $p \geqq 2$. Then $\theta_*(L\theta_*) \leqq w$ a.e. in Ω.*

Proof. We define $v_k = \theta_k - \theta_*$ such that $v_k \rightharpoonup 0$. Then it suffices to show that $v_k(Lv_k) \rightharpoonup z$ implies $0 \leqq z$.

There are two closely related ways to prove this result. The first uses the H-measure as developed in [Tar90, Ger91]: we apply Corollary 1.12 of [Tar90] to the sequences $U_{1,k} = U_{2,k} = v_k$ and the operators $A_1 = \mathrm{id}$ and $A_2 = L$ and use the positivity of the diagonal entries of the H-measure.

We describe the second proof in more detail. It is based solely on the theory of pseudo-differential operators. Let $\phi \geqq 0$ be an arbitrary localization function and denote by M_ϕ the multiplication operator $v \mapsto \phi v$. Then $M_\phi L = LM_\phi + K_\phi$ where K_ϕ is a compact operator depending only on ϕ (see, e.g., [Tar90, Lemma 1.7] and [The01]).

For a sequence $(v_k)_{k\in\mathbb{N}}$ with $v_k \rightharpoonup 0$ and $v_k\, Lv_k \rightharpoonup z$ we find that

$$\begin{aligned}\int_\Omega \phi^2\, z\,\mathrm{d}x &= \lim_{k\to\infty} \int_\Omega \phi^2\, v_k\, (Lv_k)\,\mathrm{d}x \\ &= \lim_{k\to\infty} \int_\Omega (M_\phi v_k)\, M_\phi(Lv_k)\,\mathrm{d}x \\ &= \lim_{k\to\infty} \int_\Omega (M_\phi v_k)\, L(M_\phi v_k)\,\mathrm{d}x + \lim_{k\to\infty} \int_{\mathbb{R}^d} (M_\phi v_k)\, (K_\phi v_k)\,\mathrm{d}x \\ &\geqq 0.\end{aligned}$$

In the last estimate we have used $L \geqq 0$ for the first term. The second term is 0 by the compactness of K_ϕ. Since ϕ was arbitrary, this gives the desired result. □

Remark 5.6. With the above theory we can easily construct cases where the operator L is strictly positive. If we assume that $\Gamma = \partial\Omega$ (condition (a) from above), then Fourier transform shows that

$$\langle \theta, L\theta\rangle = \int_\Omega \theta\, (L\theta)\,\mathrm{d}x = \int_{\mathbb{R}^d} \ell(\omega)|(\mathcal{F}\theta_{\mathrm{ext}})(\omega)|^2\,\mathrm{d}\omega$$

with $\theta_{\mathrm{ext}}(x) = \theta(x)$ for $x \in \Omega$ and $= 0$ for $x \in \mathbb{R}^d \setminus \Omega$. This implies $\langle \theta, L\theta\rangle > 0$ for all $\theta \neq 0$ if and only if $\ell(\omega) \neq 0$ for a.e. $\omega \in \mathbb{R}^d$. Since $\ell|_{\mathbb{S}^{d-1}}$ is analytic the latter condition holds whenever ℓ is not identically 0.

The case $\ell \equiv 0$ may occur in degenerate or highly symmetric cases. Recall that ℓ always vanishes along at least one straight line. If now the elastic tensor is isotropic and $A_2 - A_1$ is a multiple of identity, then ℓ must be rotationally symmetric and hence vanishes everywhere.

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