Universität Stuttgart
Mathematisches Institut A
1. Lehrstuhl

Angewandte Analysis
Pfaffenwaldring 57
D–70569 Stuttgart

http://www.mathematik.uni-stuttgart.de/mathA/lst1/

Nonconvex Potentials and Microstructures in Finite–Strain Plasticity

by

Carsten Carstensen

Max Planck Institute for Mathematics in the Sciences, Inselstr. 22-26, D–04103 Leipzig.
(On Leave from Mathematisches Seminar, Christian–Albrechts–Universität zu Kiel)
cc@numerik.uni-kiel.de

Klaus Hackl

Lehrstuhl für Allgemeine Mechanik, Ruhr–Universität Bochum, D–44780 Bochum.
hackl@am.bi.ruhr-uni-bochum.de

Alexander Mielke

Mathematisches Institut A, Universität Stuttgart, D–70569 Stuttgart.
mielke@mathematik.uni-stuttgart.de

NONCONVEX POTENTIALS AND MICROSTRUCTURES IN FINITE–STRAIN PLASTICITY

CARSTEN CARSTENSEN, KLAUS HACKL, AND ALEXANDER MIELKE

Abstract. A mathematical model for a finite–strain elastoplastic evolution problem is proposed in which one time–step of an implicit time–discretisation leads to generally non–convex minimisation problems. The elimination of all internal variables enables a mathematical and numerical analysis of a reduced problem within the general framework of calculus of variations and nonlinear partial differential equations. The results for a single slip–system and von Mises plasticity illustrate that finite–strain elastoplasticity generates reduced problems with non–quasiconvex energy densities and so allows for non–attainment of energy minimisers and microstructures.

1. Introduction

This paper is devoted to questions of well–posedness of problems that arise in the numerical and mathematical modelling of finite elastoplasticity; it aims to design (classes of) constitutive models (by specifying energy densities, yield functions, and hardening laws) which allow for a mathematical existence theory and, hence, for a reliable and efficient finite element approximation. The main concern is on the mathematical investigation of the variational problem in one time–increment utilising state of the art methods from the calculus of variations and, e.g., the notions rank–one convexity and quasiconvexity.

The incremental problem for elastoplasticity is a variational problem with respect to the elastic deformation as well as the plastic parameters ($\boldsymbol{F}_{\mathrm{p}}$ and the hardening parameters p). One key assumption is the design of a dissipation function which encodes the information on the yield function and depends on the new and the old plastic parameters. The functional to be minimised is the increment in the elastic (bulk) energy plus the dissipated energy.

This paper results from the authors' long–time research; models with similar ingredients have been proposed in [Lee69, Sim88, SiO85, MiS93, Mie94, OrR99]. As its main advantage, the proposed model allows for a mathematical and numerical analysis and so facilitates a theory that predicts microstructures. It appears that shear–bands, cracks, and inclusions are not bifurcation phenomena, but arise as different aspects of the same general variational model.

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A brief discussion of the model introduced in Section 2 requires further notation. Let $\boldsymbol{\phi} : \Omega \to \mathbb{R}^3$ be the deformation of a body $\Omega \subset \mathbb{R}^3$ with a deformation gradient $\boldsymbol{F} := \mathrm{D}\boldsymbol{\phi}$. Its multiplicative split $\boldsymbol{F} = \boldsymbol{F}_{\mathbf{e}}\boldsymbol{F}_{\mathbf{p}}$ into an elastic part $\boldsymbol{F}_{\mathbf{e}}$ and an irreversible, plastic part $\boldsymbol{F}_{\mathbf{p}}$ introduces the plastic parameter $\boldsymbol{P} = \boldsymbol{F}_{\mathbf{p}}^{-1}$. With an additional m–dimensional internal hardening parameter p, the stored energy density W is assumed to depend only on $\boldsymbol{F}_{\mathbf{e}} = \boldsymbol{F}\boldsymbol{P}$ and p, i.e., $W(\boldsymbol{F}, \boldsymbol{F}_{\mathbf{p}}, p) = \overline{W}(\boldsymbol{F}\boldsymbol{P}, p)$. The resulting thermo–mechanically conjugated variables [Ric71, CoG67, Hac97, HaN75, Mau92, Mor70, Mor76, ZiW87] are defined by

$$\begin{array}{ll} \boldsymbol{T} = \frac{\partial W}{\partial \boldsymbol{F}}(\boldsymbol{F}, \boldsymbol{P}, p) = \mathrm{D}_{\boldsymbol{F}_{\mathbf{e}}}\overline{W}(\boldsymbol{F}\boldsymbol{P}, p)\boldsymbol{P}^{\mathrm{T}} & \text{(first Piola–Kirchhoff stress tensor)}, \\ \boldsymbol{Q} = -\frac{\partial W}{\partial \boldsymbol{P}}(\boldsymbol{F}, \boldsymbol{P}, p) = -\boldsymbol{F}^{\mathrm{T}}\mathrm{D}_{\boldsymbol{F}_{\mathbf{e}}}\overline{W}(\boldsymbol{F}\boldsymbol{P}, p) & \text{(conjugate plastic stresses)}, \\ q = -\frac{\partial W}{\partial p}(\boldsymbol{F}, \boldsymbol{P}, p) = -\mathrm{D}_p\overline{W}(\boldsymbol{F}\boldsymbol{P}, p) & \text{(conjugate hardening forces)}. \end{array}$$

One key–point in the ansatz below is to write the variational inequalities for the irreversible deformations in terms of the mixed variant tensor $\overline{\boldsymbol{Q}}$,

$$\overline{\boldsymbol{Q}} = \boldsymbol{P}^{\mathrm{T}}\boldsymbol{Q} = -\boldsymbol{F}_{\mathbf{e}}^{\mathrm{T}}\mathrm{D}_{\boldsymbol{F}_{\mathbf{e}}}\overline{W}(\boldsymbol{F}_{\mathbf{e}}, p).$$

The yield function φ depends on q and $\overline{\boldsymbol{Q}}$ and so is invariant under plastic deformations. The principle of maximal dissipation results in the associated flow rule (which first appeared in [Mor70])

$$\begin{pmatrix} \boldsymbol{P}^{-1}\dot{\boldsymbol{P}} \\ \dot{p} \end{pmatrix} = \lambda \begin{pmatrix} \frac{\partial \varphi}{\partial \overline{\boldsymbol{Q}}}(\overline{\boldsymbol{Q}}, q) \\ \frac{\partial \varphi}{\partial q}(\overline{\boldsymbol{Q}}, q) \end{pmatrix} \quad \text{for } \varphi \le 0 \le \lambda \text{ with } \lambda\varphi = 0. \tag{1.1}$$

Using the characteristic function J with $J(\overline{\boldsymbol{Q}}, q) = 0$ for $\varphi(\overline{\boldsymbol{Q}}, q) \le 0$ and otherwise $J = \infty$, (1.1) reads $(\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}, \dot{p}) \in \partial J(\overline{\boldsymbol{Q}}, q)$ with the sub–differential ∂J of the convex function J.

A time–discretisation of the problem at hand leads typically to an elastic–plastic interactions which we aim to model as a variational problem. Given a time–discretisation $0 = t_0 < t_1 < \ldots < t_N = T$ and data $(\boldsymbol{P}_{j-1}, p_{j-1})$, Section 4 seeks the state variables $(\boldsymbol{\phi}, \boldsymbol{P}, p)$ at time t_j as minimisers of the functional $\mathcal{I}_{\boldsymbol{f}(t_j),\boldsymbol{P}_{j-1},p_{j-1}}$,

$$\begin{aligned} &\mathcal{I}_{\boldsymbol{f}(t_j),\boldsymbol{P}_{j-1},p_{j-1}}(\boldsymbol{\phi}, \boldsymbol{P}, p) = \int_\Omega \left\{\Psi(\mathrm{D}\boldsymbol{\phi}, \boldsymbol{P}, p; \boldsymbol{P}_{j-1}, p_{j-1}) - \boldsymbol{f}(t_j) \cdot \boldsymbol{\phi}\right\} \mathrm{d}\boldsymbol{x} \\ &\text{with } \Psi(\boldsymbol{F}, \boldsymbol{P}, p; \boldsymbol{P}_{j-1}, p_{j-1}) = \overline{W}(\boldsymbol{F}\,\boldsymbol{P}) + J^*(\Delta(\boldsymbol{P}_{j-1}, \boldsymbol{P}), p - p_{j-1}), \end{aligned} \tag{1.2}$$

the volume force $\boldsymbol{f}(t_j)$ at time t_j, and the Legendre transform J^* of J (cf. (4.1)); the dissipation reads $\overline{\boldsymbol{Q}} : (\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}) + q \cdot \dot{p} = J^*(\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}, \dot{p})$ and $\Delta(\boldsymbol{P}_{j-1}, \boldsymbol{P})$ approximates $\boldsymbol{P}(t_j)^{-1}\dot{\boldsymbol{P}}(t_j)$.

Amongst the main advantages of incremental problem (1.2) we stress the availability of highly developed mathematical tools for its analysis within the calculus of variations and the convenient numerical solution of a space–discretised version of (1.2). Another key–advantage is the observation in (1.2) that $\mathcal{I}_{\boldsymbol{f}(t_j),\boldsymbol{P}_{j-1},p_{j-1}}$ depends locally on the plastic variables, i.e., given $\boldsymbol{P}_{j-1}, p_{j-1}$ and a deformation gradient $\boldsymbol{F}$ and a material point $\boldsymbol{x}$ we can compute the reduced density function

$$\Psi^{\mathrm{red}}_{\boldsymbol{P}_{j-1},p_{j-1}}(\boldsymbol{x}, \boldsymbol{F}) = \min_{\boldsymbol{P},p} \Psi(\boldsymbol{F}, \boldsymbol{P}, p; \boldsymbol{P}_{j-1}(\boldsymbol{x}), p_{j-1}(\boldsymbol{x})) \tag{1.3}$$

(where minimisation is over $(\boldsymbol{P}, p) \in \mathbb{R}^{3\times3} \times \mathbb{R}^m$). Thus, (1.2) is recast into

$$\mathcal{I}^{\mathrm{red}}_{\boldsymbol{f}(t_j),\boldsymbol{P}_{j-1},p_{j-1}}(\boldsymbol{\phi}) = \int_\Omega \left\{ \Psi^{\mathrm{red}}_{\boldsymbol{P}_{j-1},p_{j-1}}(\boldsymbol{x}, \mathrm{D}\boldsymbol{\phi}) - \boldsymbol{f}(t_j) \cdot \boldsymbol{\phi} \right\} \mathrm{d}\boldsymbol{x}. \tag{1.4}$$

The proposed model (1.4) focuses the analysis to the reduced functional $\mathcal{I}^{\mathrm{red}}$ of the form as in nonlinear elasticity. As a consequence, we analyse the rank–one convexity of the reduced density function $\Psi^{\mathrm{red}}_{\boldsymbol{P}_0,p_0}(\boldsymbol{x},\cdot) : \mathbb{R}^{3\times3} \to \mathbb{R}$ which depends via $\overline{W}$ and J^* simultaneously on the elastic and the plastic properties of the material.

Two particular examples illustrate consequences of the theory proposed; both represent typical models used in the mechanics of materials. The first describes an elastoplastic single crystal with one active slip–system, the second is the finite–strain version of the well–known von Mises model for polycrystalline metals. In both cases, the reduced density function is not quasiconvex which indicates the occurrence of microstructures in the associated plasticity models. Indeed such microstructures have been observed experimentally, [Kor98, Per98, OrR99]. The common formulations based on evolution equations for the internal variables (flow rules), however, have only been able to explain the occurrence of shear bands (singularities of the deformation field) but have failed to predict more complex structures ([OrR99] makes an attempt in this direction for crystal plasticity). The theory presented here is in principle able to describe microstructures in their full complexity by transforming evolution equations into an optimisation problem. Two further results might be worth mentioning here as they are contradictory to common belief: (a) Finite–strain von Mises plasticity does not reduce to the Prandtl–Reuss model in the small–strain limit. (b) Substantial amount of hardening is required in order to render the model quasiconvex.

The remainder of this paper is organised as follows. Section 2 recalls standard concepts in finite–strain continuum mechanics and introduces the time–continuous model for elastoplastic evolution. The incremental problem is established in Section 3 for a class of implicit time–discretisations and then recast into an incremental minimisation problem in Section 4. Eventually the internal variables are eliminated and so the reduced problem is established in Section 5. The final two sections illustrate this reduction procedure for two specific plasticity models, a single slip–system and von Mises elastoplasticity. In both cases, the reduced density function is not quasiconvex which predicts microstructure in the associated plasticity models.

2. Rate–independent elastoplasticity

This section establishes the (time–continuous) model of elastoplastic evolution in continuum mechanics. The deformation $\boldsymbol{\phi} : \Omega \to \mathbb{R}^d$ of a body $\Omega \subset \mathbb{R}^d$ (where $d = 1, 2,$ or 3) is a mapping with a (distributional) gradient $\boldsymbol{F}(\boldsymbol{x}) = \mathrm{D}_{\boldsymbol{x}}\boldsymbol{\phi}(\boldsymbol{x}) \in \mathbb{R}^{d\times d}$ of positive determinant for (almost each) $\boldsymbol{x} \in \Omega$. Usual italics denote scalar functions or n–tuples, lower case bold face letters indicate vectors and co–vectors ($\boldsymbol{x}$, $\boldsymbol{\phi}$, $\dots$), and uppercase boldface letters describe tensors ($\boldsymbol{F}, \boldsymbol{T}, \dots$). All the subsequent notation is consistent with the general notions of the analysis on manifolds, but we do not employ these concepts and regard tensors as matrices and so utilise standard matrix algebra.

Our model of quasi–static elastoplasticity is deduced from two basic principles: The *equilibrium equation* is derived by energy minimisation (or stationary states) with respect to variations of $\boldsymbol{\phi}$ and the plastic flow rule is derived from the *principle of maximum plastic dissipation.* Certain options of relevant plastic strains are possible and amongst several options of relevant plastic strains, our choice reflects invariance properties and is based on the hypothesis that the elastic energy and the yield stresses are independent of the plastic deformation.

The plastic behaviour is given through the multiplicative split $\boldsymbol{F} = \boldsymbol{F}_{\mathbf{e}}\boldsymbol{F}_{\mathbf{p}}$ of $\boldsymbol{F}$ into an elastic part $\boldsymbol{F}_{\mathbf{e}}$ and the plastic part $\boldsymbol{F}_{\mathbf{p}}$; $\boldsymbol{F}_{\mathbf{e}}$ and $\boldsymbol{F}_{\mathbf{p}}$ are invertible with their product $\boldsymbol{F}$, written $\boldsymbol{F}$, $\boldsymbol{F}_{\mathbf{e}}$, $\boldsymbol{F}_{\mathbf{p}} \in \mathsf{GL}(d)$. The material properties may depend on internal plastic variables $p \in \mathbb{R}^m$ (such as hardening parameters) and so the internal stored energy is postulated in the form

$$W(\boldsymbol{F}, \boldsymbol{F}_{\mathbf{p}}, p) = \overline{W}(\boldsymbol{F}\boldsymbol{F}_{\mathbf{p}}^{-1}, p) = \overline{W}(\boldsymbol{F}_{\mathbf{e}}, p). \tag{2.1}$$

In the sequel, we will use the plastic variables $(\boldsymbol{P}, p)$ with the plastic configuration change $\boldsymbol{P} = \boldsymbol{F}_{\mathbf{p}}^{-1}$. The assumption that the elastic energy depends only on the elastic part of the deformation gradient is essential in our analysis and is motivated by the observation that plastic deformation results from a configurational change of the material body (dislocation movements in the case of metal plasticity): Plastic deformation simply recasts the reference configuration into another one and so does not affect the elastic deformation. For details see, e.g., [Hac97, Mau92, Sim88, Mie94].

Material objectivity requires $\overline{W}(\boldsymbol{R}\boldsymbol{F}_{\mathrm{e}}, p) = \overline{W}(\boldsymbol{F}_{\mathrm{e}}, p)$ for all $\boldsymbol{R} \in \mathrm{SO}(d)$ or, equivalently,

$$\overline{W}(\boldsymbol{F}_{\mathbf{e}}, p) = \widehat{W}(\boldsymbol{F}_{\mathbf{e}}^{\mathrm{T}}\boldsymbol{F}_{\mathbf{e}}, p),$$

where $^{\mathrm{T}}$ denotes the transposed matrix (in Cartesian coordinates assumed).

In rate–independent elastoplasticity, the body is in equilibrium for each instant (of the process time $t \in [0, T]$). This specifies the deformation $\boldsymbol{\phi}$ as soon as the evolution of the plastic variables $\boldsymbol{P} = \boldsymbol{F}_{\mathbf{p}}^{-1}$ and p is given. The thermo–mechanical dual variables read

$$\boldsymbol{T} = \frac{\partial W}{\partial \boldsymbol{F}}, \quad \boldsymbol{Q} = -\frac{\partial W}{\partial \boldsymbol{F}_{\mathbf{p}}^{-1}}, \quad q = -\frac{\partial W}{\partial p}.$$

Here $\boldsymbol{T}$ is the first Piola–Kirchhoff stress tensor and $\boldsymbol{Q}$ contains the plastic (back-) stresses. The minus sign in the definitions of $\boldsymbol{Q}$ and q follows standard conventions, in particular in elastoplasticity using the linearised strain tensor, see [Suq81, Suq88, HaR95]. For the special ansatz (2.1) we obtain

$$\boldsymbol{T} = \mathrm{D}_{\boldsymbol{F}_{\mathbf{e}}}\overline{W}(\boldsymbol{F}_{\mathrm{e}}, p)\boldsymbol{P}^{\mathrm{T}}, \quad \boldsymbol{Q} = -\boldsymbol{F}^{\mathrm{T}}\mathrm{D}_{\boldsymbol{F}_{\mathbf{e}}}\overline{W}(\boldsymbol{F}_{\mathrm{e}}, p), \quad q = -\mathrm{D}_p\overline{W}(\boldsymbol{F}_{\mathrm{e}}, p). \tag{2.2}$$

The evolution of $(\boldsymbol{P}, p)$ is governed by a flow rule associated with the yield function φ via the principle of maximum plastic dissipation. In general, φ depends on the stresses $\boldsymbol{T}$, $\boldsymbol{Q}$, and q. However, our second postulate (in addition to (2.1)) is that the yield function φ is independent of the plastic deformation $\boldsymbol{F}_{\mathbf{p}} = \boldsymbol{P}^{-1}$. From (2.2) we see that the tensor

$$\overline{\boldsymbol{Q}} = \boldsymbol{P}^{\mathrm{T}}\boldsymbol{Q} = -\boldsymbol{F}_{\mathbf{e}}^{\mathrm{T}}\mathrm{D}_{\boldsymbol{F}_{\mathbf{e}}}\overline{W}(\boldsymbol{F}_{\mathbf{e}}, p)$$

is invariant under all plastic deformations and hence we postulate that the yield function depends on $\overline{\boldsymbol{Q}}$ and q only,

$$\varphi(\boldsymbol{T}, \boldsymbol{Q}, q) = \overline{\varphi}(\overline{\boldsymbol{Q}}, q) = \overline{\varphi}(\boldsymbol{P}^{\mathrm{T}}\boldsymbol{Q}, q). \tag{2.3}$$

The yield function defines the set of admissible stresses

$$\mathbb{Q} \stackrel{\text{def}}{=} \{\, (\overline{\boldsymbol{Q}}, q) \in \mathbb{R}^{d\times d} \times \mathbb{R}^m \;:\; \varphi(\overline{\boldsymbol{Q}}, q) \le 0 \,\}$$

and we assume that $\mathbb{Q}$ is convex and contains $(\mathbf{0}, 0)$. The characteristic function of $\mathbb{Q}$ is

$$J(\boldsymbol{Q}, q) \stackrel{\text{def}}{=} \begin{cases} 0 & \text{for } (\boldsymbol{Q}, q) \in \mathbb{Q}, \\ \infty & \text{else.} \end{cases}$$

The principle of *maximal plastic dissipation* [Sim88] postulates that the plastic dissipation

$$-\mathrm{D}_{\boldsymbol{P}}W(\boldsymbol{F}, \boldsymbol{P}, p) : \dot{\boldsymbol{P}} - \mathrm{D}_p W(\boldsymbol{F}, \boldsymbol{P}, p) \cdot \dot{p} = \boldsymbol{Q} : \dot{\boldsymbol{P}} + q \cdot p = \overline{\boldsymbol{Q}} : (\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}) + q \cdot \dot{p}.$$

is maximal when the rates $\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}$ and $\dot{p}$ are kept fixed and the stresses $(\boldsymbol{Q}, q)$ are varied in $\mathbb{Q}$. This leads to

$$\overline{\boldsymbol{Q}} : (\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}) + q \cdot \dot{p} \ge \boldsymbol{S} : (\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}) + s \cdot \dot{p} \quad \text{for all } (\boldsymbol{S}, s) \in \mathbb{Q}. \tag{2.4}$$

Using the definition of J and its sub–differential

$$\partial J(\overline{\boldsymbol{Q}}, q) = \big\{ (\overline{\boldsymbol{P}}, \overline{p}) \in \mathbb{R}^{d\times d} \times \mathbb{R}^m \;:\; \begin{array}{l} J(\overline{\boldsymbol{Q}} + \boldsymbol{S}, q + s) \ge J(\overline{\boldsymbol{Q}}, q) + \overline{\boldsymbol{P}} : \boldsymbol{S} + \overline{p} \cdot s \\ \text{for all } (\boldsymbol{S}, s) \in \mathbb{R}^{d\times d} \times \mathbb{R}^m \big\}, \end{array}$$

the principle of maximum dissipation (2.4) reads

$$(\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}, \dot{p}) \in \partial J(\overline{\boldsymbol{Q}}, q). \tag{2.5}$$

The above constitutive functions $\overline{W}$ and $\overline{\varphi}$ result in a total elastoplastic problem we only formulate for pure displacement boundary conditions (changes necessary for traction boundary conditions are standard).

Elastoplastic problem. Given the (volume) forces $\boldsymbol{f} : [0,T] \times \Omega \to \mathbb{R}^d$, the boundary data $\boldsymbol{\phi}_{\mathrm{bc}} : [0,T] \times \partial\Omega \to \mathbb{R}^d$, the initial conditions for the plastic variables $(\boldsymbol{P}_0, p_0) : \Omega \to \mathsf{GL}(d) \times \mathbb{R}^m$; find a deformation $\boldsymbol{\phi} : [0,T] \times \Omega \to \mathbb{R}^d$ and plastic variables $(\boldsymbol{P}, p) : [0,T] \times \Omega \to \mathsf{GL}(d) \times \mathbb{R}^m$ satisfying

$$\begin{aligned}
&\text{(equilibrium)} && \operatorname{div} \boldsymbol{T} + \boldsymbol{f} = 0 \quad \text{for } (t,\boldsymbol{x}) \in [0,T] \times \Omega,\\
&\text{(flow rule)} && (\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}, \dot{p}) \in \partial J(\overline{\boldsymbol{Q}}, q) \quad \text{for } (t,\boldsymbol{x}) \in [0,T] \times \Omega,\\
&\text{(deformation gradient)} && \boldsymbol{F} = \mathrm{D}_{\boldsymbol{x}} \boldsymbol{\phi},\\
&\text{(constitutive laws)} && \boldsymbol{T} = \mathrm{D}_{\boldsymbol{F}_\mathsf{e}} \overline{W}(\boldsymbol{F}\boldsymbol{P}, p) \boldsymbol{P}^{\mathrm{T}},\\
& && \overline{\boldsymbol{Q}} = -(\boldsymbol{F}\boldsymbol{P})^{\mathrm{T}} \mathrm{D}_{\boldsymbol{F}_\mathsf{e}} \overline{W}(\boldsymbol{F}\boldsymbol{P}, p), \ q = -\mathrm{D}_{\boldsymbol{F}_\mathsf{e}} \overline{W}(\boldsymbol{F}\boldsymbol{P}, p),\\
&\text{(initial conditions)} && \boldsymbol{P}(0,\boldsymbol{x}) = \boldsymbol{P}_0(\boldsymbol{x}), \ p(0,\boldsymbol{x}) = p_0(\boldsymbol{x}) \text{ for } \boldsymbol{x} \in \Omega,\\
&\text{(boundary conditions)} && \boldsymbol{\phi}(t,\boldsymbol{x}) = \boldsymbol{\phi}_{\mathrm{bc}}(t,\boldsymbol{x}) \text{ for } (t,\boldsymbol{x}) \in [0,T] \times \partial\Omega.
\end{aligned}$$

Remark 2.1. Note that $\overline{\boldsymbol{Q}}$ can be understood as a linear operator from the cotangent bundle of the intermediate configuration into itself and thus the invariants like eigenvalues, determinant and the trace are well defined [Hac97].

Remark 2.2. Formulations of the type (2.3) and (2.5) have been used first in the context of small–strain elastoplasticity by [Mor70] and [HaN75].

3. Time–discrete formulation

This section concerns two time–discretisations to emphasise that their choice within the flow–rule is non–unique. Mathematical proofs of existence of solutions or their numerical approximation are based on the understanding of one time–increment. Assume that the time interval $[0,T]$ is discretised into $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$ and that approximations $(\boldsymbol{\phi}_j, \boldsymbol{P}_j, p_j)$ for $(\boldsymbol{\phi}(t_j,\cdot), \boldsymbol{P}(t_j,\cdot), p(t_j,\cdot))$ are known for $j = 1, \ldots, k$. The incremental problem is to find approximations at the time level t_{k+1}. Since this problem is of the same type for all $k = 0, 1, 2, \ldots, n-1$, we will restrict the notation to the first step, i.e., $k = 0$, and so $(\boldsymbol{P}_0, p_0)$, $(\boldsymbol{P}, p) = (\boldsymbol{P}_1, p_1)$ and $\tau = t_1 - t_0$. As the only link between the time levels are the derivatives in the flow rule we have to discretise these derivatives.

In contrast to the straightforward discretisation of the derivative $\dot{p} \approx \frac{1}{\tau}(p - p_0)$, the discretisation $\frac{1}{\tau}\Delta(\boldsymbol{P}, \boldsymbol{P}_0)$ of $\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}$ at $t = t_1$ offers various possible realisations, for instance

$$\Delta(\boldsymbol{P}, \boldsymbol{P}_0) = (\theta \boldsymbol{P}_0 + (1-\theta)\boldsymbol{P})^{-1}(\boldsymbol{P} - \boldsymbol{P}_0) \text{ or } \Delta(\boldsymbol{P}, \boldsymbol{P}_0) = (\theta \boldsymbol{P}_0^{-1} + (1-\theta)\boldsymbol{P}^{-1})(\boldsymbol{P} - \boldsymbol{P}_0).$$

Both cases coincide for $\theta = 0$ or 1. For $\theta = 0$ the approximation is linear in $\boldsymbol{P}$, and for $\theta = 1$ it is linear in $\boldsymbol{P}^{-1}$. Another possibility is $\Delta(\boldsymbol{P}_0, \boldsymbol{P}) = \log(\boldsymbol{P}_0^{-1}\boldsymbol{P})$ which rather corresponds to the multiplicative decomposition. The only restriction reads

$$\Delta(\boldsymbol{P}_0, \boldsymbol{P}_0(\boldsymbol{1} + \boldsymbol{S})) = \boldsymbol{S} + \mathcal{O}(|\boldsymbol{S}|^2) \text{ for } \boldsymbol{S} \to \boldsymbol{0}. \tag{3.1}$$

Incremental problem. Given the (volume) forces $\boldsymbol{f}:\Omega\to\mathbb{R}^d$, the boundary data $\boldsymbol{\phi}_{\mathrm{bc}}:\partial\Omega\to\mathbb{R}^d$ and the initial conditions for the plastic variables $(\boldsymbol{P}_0,p_0):\Omega\to\mathsf{GL}(d)\times\mathbb{R}^m$; find the deformation $\boldsymbol{\phi}:\Omega\to\mathbb{R}^d$, the plastic variables $(\boldsymbol{P},p):\Omega\to\mathsf{GL}(d)\times\mathbb{R}^m$ such that the following holds

$$
\begin{aligned}
&\text{(equilibrium)} && \operatorname{div}\boldsymbol{T}+\boldsymbol{f}=0 \quad \text{for } \boldsymbol{x}\in\Omega,\\
&\text{(discretised flow rule)} && (\Delta(\boldsymbol{P}_0,\boldsymbol{P}),p-p_0)\in\partial J(\overline{\boldsymbol{Q}},q) \quad \text{for } \boldsymbol{x}\in\Omega,\\
&\text{(deformation gradient)} && \boldsymbol{F}=\mathrm{D}_{\boldsymbol{x}}\boldsymbol{\phi},\\
&\text{(constitutive laws)} && \boldsymbol{T}=\mathrm{D}_{\boldsymbol{F}_{\mathsf{e}}}\overline{W}(\boldsymbol{F}\boldsymbol{P},p)\boldsymbol{P}^{\mathrm{T}},\\
& && \overline{\boldsymbol{Q}}=-(\boldsymbol{F}\boldsymbol{P})^{\mathrm{T}}\mathrm{D}_{\boldsymbol{F}_{\mathsf{e}}}\overline{W}(\boldsymbol{F}\boldsymbol{P},p),\ q=-\mathrm{D}_{\boldsymbol{F}_{\mathsf{e}}}\overline{W}(\boldsymbol{F}\boldsymbol{P},p),\\
&\text{(boundary conditions)} && \boldsymbol{\phi}(\boldsymbol{x})=\boldsymbol{\phi}_{\mathrm{bc}}(\boldsymbol{x}) \text{ for } \boldsymbol{x}\in\partial\Omega.
\end{aligned}
$$

Remark 3.1. This paper focuses on the solvability of the incremental steps in the time–discretisation of the time continuous problem; convergence questions for smaller and smaller increments are beyond this paper. A result in this direction was obtained in [MTL00] for a rate–independent flow–rule model for phase transformations in shape memory alloys.

4. Variational formulation

This section is devoted to recast the incremental problem into a minimisation problem. Given $\boldsymbol{\phi}_{\mathrm{bc}}, \boldsymbol{f}, \boldsymbol{P}_0$, and p_0 we associate the functional

$$I(\boldsymbol{\phi},\boldsymbol{P},p,\overline{\boldsymbol{Q}},q)=\int_\Omega\Big[\overline{W}(\mathrm{D}_{\boldsymbol{x}}\boldsymbol{\phi}\boldsymbol{P},p)-\boldsymbol{f}\cdot\boldsymbol{\phi}+\overline{\boldsymbol{Q}}:\Delta(\boldsymbol{P}_0,\boldsymbol{P})+q\cdot(p-p_0)-\tau J(\overline{\boldsymbol{Q}},q)\Big]\,\mathrm{d}\boldsymbol{x}$$

and study its derivatives. A variation with respect to $\boldsymbol{\phi}$ (under the given boundary conditions) yields

$$\operatorname{div}\boldsymbol{T}+\boldsymbol{f}=0 \text{ with } \boldsymbol{T}=\mathrm{D}_{\boldsymbol{F}_{\mathsf{e}}}\overline{W}(\mathrm{D}_{\boldsymbol{x}}\boldsymbol{\phi}\boldsymbol{P})\boldsymbol{P}^{\mathrm{T}},$$

i.e., the equilibrium and the constitutive law for the kinematic stress tensor. A variation with respect to the dual variables $(\overline{\boldsymbol{Q}},q)$ gives exactly the discretised flow rule

$$\frac{1}{\tau}(\Delta(\boldsymbol{P}_0,\boldsymbol{P}),p-p_0)\in\partial J(\overline{\boldsymbol{Q}},q).$$

A variation with respect to the plastic hardening variables p yields the constitutive relation for q,

$$\mathrm{D}_p\overline{W}(\mathrm{D}_{\boldsymbol{x}}\boldsymbol{\phi}\boldsymbol{P},p)+q=0.$$

A variation of I with respect to $\boldsymbol{P}$ depends on the choice in (3.1) and we discuss two cases

$$\Delta_1(\boldsymbol{P}_0,\boldsymbol{P})=\boldsymbol{P}_0^{-1}\boldsymbol{P}-\mathbf{1} \quad \text{resp.} \quad \Delta_2(\boldsymbol{P}_0,\boldsymbol{P})=\mathbf{1}-\boldsymbol{P}^{-1}\boldsymbol{P}_0.$$

which are either linear in $\boldsymbol{P}$ or in $\boldsymbol{P}^{-1}$. A variation of I with respect to $\boldsymbol{P}$ yields

$$-\boldsymbol{F}^{\mathrm{T}}\mathrm{D}_{\boldsymbol{F}_{\mathrm{e}}}\overline{W}(\boldsymbol{F}_{\mathrm{e}},p)=\begin{cases}(\boldsymbol{P}_0^{-1})^{\mathrm{T}}\overline{\boldsymbol{Q}} & \text{for } \Delta_1,\\ (\boldsymbol{P}_0^{-1})^{\mathrm{T}}\overline{\boldsymbol{Q}}(\boldsymbol{P}^{-1}\boldsymbol{P}_0)^{\mathrm{T}} & \text{for } \Delta_2,\end{cases}$$

as an approximation of the constitutive relation of $\overline{\boldsymbol{Q}}$. Hence the preceding incremental problem has essentially the structure of a constitutive relation for $\overline{\boldsymbol{Q}}$.

In summary, stationary points of I can be obtained by maximising with respect to $(\overline{\boldsymbol{Q}},q)$ and minimisation with respect to the remaining variables.

Proposition 4.1. *A stationary point of the functional I solves the incremental problem of Section 3.* □

The task to find stationary points of I is rewritten by utilising the Legendre transform J^*,

$$\begin{aligned} J^*(\boldsymbol{S},s) &= \sup\left\{\,\overline{\boldsymbol{Q}}:\boldsymbol{S}+q\cdot s-J(\overline{\boldsymbol{Q}},q)\ :\ (\overline{\boldsymbol{Q}},q)\in\mathbb{R}^{d\times d}\times\mathbb{R}^m\,\right\}\\ &= \sup\left\{\,\overline{\boldsymbol{Q}}:\boldsymbol{S}+q\cdot s\ :\ (\overline{\boldsymbol{Q}},q)\in\mathbb{Q}\,\right\}, \end{aligned} \tag{4.1}$$

of J. Recall from convex analysis [Zei85] that, the subgradients of J and J^* are linked,

$$(\boldsymbol{S},s)\in\partial J(\overline{\boldsymbol{Q}},q)\iff(\overline{\boldsymbol{Q}},q)\in\partial J^*(\boldsymbol{S},s).$$

Since J assumes only the values 0 and ∞, the function J^* is homogeneous of degree 1, that is $J^*(\alpha(\boldsymbol{S},s))=\alpha J^*(\boldsymbol{S},s)$ for all $\alpha\geq 0$. Moreover, $J^*(\boldsymbol{S},s)\geq 0$ because of $(\boldsymbol{0},0)\in\mathbb{Q}$ and $\partial J^*((\boldsymbol{0},0))=\mathbb{Q}$. Hence a maximisation of I with respect to $(\overline{\boldsymbol{Q}},q)$ leads to the functional

$$\begin{aligned} &\mathcal{I}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\boldsymbol{\phi},\boldsymbol{P},p)=\int_\Omega\Psi(\boldsymbol{x},\mathrm{D}\boldsymbol{\phi}(\boldsymbol{x}),\boldsymbol{P}(\boldsymbol{x}),p(\boldsymbol{x});\boldsymbol{P}_0(\boldsymbol{x}),p_0(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x}-\ell(\boldsymbol{\phi}),\\ &\text{where } \Psi(\boldsymbol{x},\boldsymbol{F},\boldsymbol{P},p;\boldsymbol{P}_0,p_0)=\overline{W}(\boldsymbol{F}\boldsymbol{P},p)+J^*(\Delta(\boldsymbol{P}_0,\boldsymbol{P}),p-p_0)\\ &\text{and } \ell(\boldsymbol{\phi})=\int_\Omega\boldsymbol{f}(\boldsymbol{x})\cdot\boldsymbol{\phi}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}. \end{aligned} \tag{4.2}$$

The incremental problem can be recast into a (equivalent) minimisation problem.

Incremental minimisation problem. Given the (volume) forces $\boldsymbol{f}:\Omega\to\mathbb{R}^d$, the boundary data $\boldsymbol{\phi}_{\mathrm{bc}}:\partial\Omega\to\mathbb{R}^d$ and the initial conditions for the plastic variables $(\boldsymbol{P}_0,p_0):\Omega\to\mathsf{GL}(d)\times\mathbb{R}^m$, find a deformation $\boldsymbol{\phi}:\Omega\to\mathbb{R}^d$ and plastic variables $(\boldsymbol{P},p):\Omega\to\mathsf{GL}(d)\times\mathbb{R}^m$ which satisfy

$$\mathcal{I}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\boldsymbol{\phi},\boldsymbol{P},p)=\inf\left\{\,\mathcal{I}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\widetilde{\boldsymbol{\phi}},\widetilde{\boldsymbol{P}},\widetilde{p})\ :\ \widetilde{\boldsymbol{\phi}},\widetilde{\boldsymbol{P}},\widetilde{p}\text{ admissible }\right\}. \tag{4.3}$$

Proposition 4.2. *If $(\boldsymbol{\phi},\boldsymbol{P},p)$ solves the incremental minimisation problem (4.3), then there exists $(\overline{\boldsymbol{Q}},q)$ in $\partial J^*(\Delta(\boldsymbol{P}_0,\boldsymbol{P}),p-p_0)$ such that $(\boldsymbol{\phi},\boldsymbol{P},p,\overline{\boldsymbol{Q}},q)$ is a stationary point of I.* □

Remark 4.3. This minimisation formulation of the incremental problem is the basis of our subsequent analysis. It allows an instructive interpretation within the realm of *material* or *Eshelbyan mechanics* [Mau93]. Here $\boldsymbol{P}$ and p play the role of a material configurational change, in our case of dislocation movement, whereas J^* specifies an incremental energy release caused by configurational changes enforced by an energy release higher than the invested elastic energy. The stress $\boldsymbol{Q} = \frac{\partial W}{\partial \boldsymbol{P}}$ is a thermodynamic driving force for configurational change called Eshelby–tensor. Similar interpretations are also possible for models involving material damage and phase transformations ([MTL99, MTL00]).

5. Reduction via pointwise minimisation

This section is devoted to a further reduction of the incremental minimisation problem owing to its structure. The internal variables $\boldsymbol{P}$ and p appear locally under the integral such that the minimisation with respect to these variables can be performed pointwise. This defines the reduced density and the reduced density function

$$\Psi^{\text{red}}_{\boldsymbol{P}_0,p_0}(\boldsymbol{x},\boldsymbol{F}) = \min\left\{\Psi(\boldsymbol{x},\boldsymbol{F},\boldsymbol{P},p;\boldsymbol{P}_0(\boldsymbol{x}),p_0(\boldsymbol{x}))\;\middle|\;(\boldsymbol{P},p)\in\mathsf{GL}(d)\times\mathbb{R}^m\right\}, \tag{5.1}$$
$$\mathcal{I}^{\text{red}}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\boldsymbol{\phi}) = \int_\Omega \Psi^{\text{red}}_{\boldsymbol{P}_0,p_0}(\boldsymbol{x},\mathrm{D}\boldsymbol{\phi}(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x} - \ell(\boldsymbol{\phi}).$$

Reduced incremental minimisation problem. Given the (volume) forces $\boldsymbol{f}:\Omega\to\mathbb{R}^d$, the boundary data $\boldsymbol{\phi}_{\text{bc}}:\partial\Omega\to\mathbb{R}^d$ and the initial conditions for the plastic variables $(\boldsymbol{P}_0,p_0):\Omega\to\mathsf{GL}(d)\times\mathbb{R}^m$, find a deformation $\boldsymbol{\phi}:\Omega\to\mathbb{R}^d$ which satisfies

$$\mathcal{I}^{\text{red}}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\boldsymbol{\phi}) = \inf\left\{\,\mathcal{I}^{\text{red}}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\widetilde{\boldsymbol{\phi}})\;:\;\widetilde{\boldsymbol{\phi}}\text{ admissible }\right\}. \tag{5.2}$$

Proposition 5.1. *The first component $\boldsymbol{\phi}$ of a minimiser $(\boldsymbol{\phi},\boldsymbol{P},p)$ of the functional $\mathcal{I}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}$ in (4.3) is a minimiser of the reduced functional $\mathcal{I}^{\text{red}}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}$. Conversely, for every minimiser $\boldsymbol{\phi}$ of the reduced functional there exists $(\boldsymbol{P},p)$ such that $(\boldsymbol{\phi},\boldsymbol{P},p)$ minimises $\mathcal{I}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}$.*

Proof. The first inclusion is a direct consequence of the preceding construction and, for the second, consider $(\boldsymbol{P}(\boldsymbol{x}),p(\boldsymbol{x}))$ such that the minimum in (5.1) is attained when $\boldsymbol{F}$ is replaced by $\mathrm{D}\boldsymbol{\phi}(\boldsymbol{x})$. □

The minimisation problem (5.2) is of the form well–analysed in nonlinear elasticity [Bal77, Dac89]. The question of existence of minimisers is in general nontrivial as the functionals are nonconvex.

Sufficient conditions for the existence of minimisers are the weak lower semicontinuity and the coercivity of the functional. The appendix gives their precise definitions and discusses the relation to the notion of cross–quasiconvexity. It turns out that the reduction step (elimination of the local plastic variables) is indeed necessary (in the sense that the detection of non–attainment is otherwise unclear).

In the following sections, two illustrative examples are addressed where the functional (5.2) is explicitly constructed. In both cases, the essential condition is rank–one convexity which is violated and so microstructure cannot be excluded.

Definition 5.2 (rank–one convexity). *The function $\psi : \mathbb{R}^{d\times d} \to \mathbb{R}$ is called rank–one convex if for every $\boldsymbol{F} \in \mathbb{R}^{d\times d}$ and $\boldsymbol{n}, \boldsymbol{m} \in \mathbb{R}^d$ the function $t \mapsto \psi(\boldsymbol{F} + t\,\boldsymbol{n} \otimes \boldsymbol{m})$ is convex on $\mathbb{R}$.*

Every quasiconvex function is rank–one convex [Dac89] and attainment of minimisers is (for the examples below) equivalent to quasiconvexity. Hence, the next sections are concerned with examples and the question if (and for which parameters) the reduced density function is rank–one convex.

6. A single slip–system

This section investigates the presented framework in the particular example of a single slip–system which models elastoplastic single crystals [Asa83], but also describes the material behaviour of ice respectively snow [GoH98], or can be applied to problems in soil mechanics.

Let $U : \mathbb{R}_+ \to \mathbb{R}$ be convex and $a > 0$ be a hardening modulus. Then, the energy density for compressible neo–Hooke material [Cia88] reads

$$\overline{W}(\boldsymbol{F}_{\mathbf{e}}, p) = U(\det \boldsymbol{F}_{\mathbf{e}}) + \frac{\mu}{2}\,\mathrm{tr}\,\boldsymbol{F}_{\mathbf{e}}^{\mathrm{T}}\boldsymbol{F}_{\mathbf{e}} + \frac{a}{2}\,p^2, \tag{6.1}$$

where $\mu > 0$ is a Lamé parameter.

Two orthogonal unit–vectors $\boldsymbol{m}$ and $\boldsymbol{n}$ ($|\boldsymbol{m}| = 1 = |\boldsymbol{n}|$, $\boldsymbol{m} \cdot \boldsymbol{n} = 0$) characterise the yield function

$$\overline{\varphi}(\overline{\boldsymbol{Q}}, q) = |\boldsymbol{m} \cdot \overline{\boldsymbol{Q}}\,\boldsymbol{n}| - r - q. \tag{6.2}$$

With a non–negative plastic consistency (slip–rate) parameter $\dot{\lambda} \geq 0$, the flow rule reads

$$\left(\boldsymbol{P}^{-1}\dot{\boldsymbol{P}}, \dot{p}\right) = \dot{\lambda}\,\left(\mathrm{sign}(\boldsymbol{m} \cdot \overline{\boldsymbol{Q}}\,\boldsymbol{n})\,\boldsymbol{m} \otimes \boldsymbol{n}, -1\right). \tag{6.3}$$

Let $\dot{\gamma} = \dot{\lambda}\,\mathrm{sign}(\boldsymbol{m} \cdot \overline{\boldsymbol{Q}}\,\boldsymbol{n})$ with $\gamma(0) = 0$. Notice that, by (6.3), $\dot{p} = -|\dot{\gamma}|$. From (6.3), $\dot{\boldsymbol{P}} = \dot{\gamma}(\boldsymbol{P}\boldsymbol{m}) \otimes \boldsymbol{n}$ and so $\boldsymbol{m} \perp \boldsymbol{n}$ yields $\dot{\boldsymbol{P}}\boldsymbol{m} = 0$. This, the initial condition $\boldsymbol{P}_0 = \mathbf{1}$, and a time–integration show $\boldsymbol{P}\boldsymbol{m} = \boldsymbol{m}$ and so $\dot{\boldsymbol{P}} = \dot{\gamma}\,\boldsymbol{m} \otimes \boldsymbol{n}$. From this, the initial condition $\boldsymbol{P}_0 = \mathbf{1}$, and by time–integration we infer

$$\boldsymbol{P} = \mathbf{1} + \gamma\,\boldsymbol{m} \otimes \boldsymbol{n}. \tag{6.4}$$

Therefore, the evolution of the internal variables $\boldsymbol{P}$ and p can essentially be described in terms of the single parameter γ. The kinematics of plastic flow is a simple shear in the plane spanned by $\boldsymbol{m}$ and $\boldsymbol{n}$. For this reason $\boldsymbol{m}$ and $\boldsymbol{n}$ are called the *slip–system.*

Direct calculations provide the Legendre–transform J^* of J,

$$\begin{aligned}
J^*(\sigma,s) &= \sup\left\{ \overline{\boldsymbol{Q}} : (\sigma\,\boldsymbol{m}\otimes\boldsymbol{n}) + qs \;:\; |\boldsymbol{m}\cdot\overline{\boldsymbol{Q}}\boldsymbol{n}| - q \le r,\ q\ge 0 \right\}\\
&= \sup\left\{ Q\sigma + qs \;:\; |Q| - q \le r,\ q\ge 0 \right\}\\
&= \sup\left\{ |Q||\sigma| + qs \;:\; |Q| - q \le r,\ q\ge 0 \right\}\\
&= \sup\left\{ (|Q|-q)|\sigma| + q(|\sigma|+s) \;:\; |Q| - q \le r,\ q\ge 0 \right\}\\
&= \sup\left\{ r|\sigma| + q(|\sigma|+s) \;:\; q\ge 0 \right\}\\
&= \begin{cases} r|\sigma| & \text{if} \quad |\sigma|+s\le 0,\\ \infty & \text{else.}\end{cases}
\end{aligned}$$

By substituting (6.4) with $\boldsymbol{F} = \boldsymbol{F}_{\mathbf{e}}\boldsymbol{P}^{-1}$ into (6.1) and making use of $\det \boldsymbol{P} = 1$ (an immediate consequence of (6.4)) we obtain a reduced functional

$$\begin{aligned}
\overline{\mathcal{I}}_{\boldsymbol{f},\gamma_0,p_0}(\boldsymbol{\phi},\gamma,p) = \int_\Omega \Big\{ & U(\det \boldsymbol{F}) + \tfrac{\mu}{2}(\operatorname{tr}\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} + 2\gamma C_{mn} + \gamma^2 C_{mm})\\
& + \tfrac{a}{2}\,p^2 + r|\gamma-\gamma_0| - \boldsymbol{f}\cdot\boldsymbol{\phi}\Big\}\,\mathrm{d}\boldsymbol{x},
\end{aligned}$$

under the constraint

$$|\gamma-\gamma_0| + p - p_0 \le 0.$$

Here, $C_{mm} = \boldsymbol{m}\cdot\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\boldsymbol{m}$ and $C_{mn} = \boldsymbol{m}\cdot\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}\boldsymbol{n}$ denote the components of the Cauchy–Green strain–tensor $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F}$ in the directions given by $\boldsymbol{m}$ and $\boldsymbol{n}$.

Minimisation with respect to p gives $p = p_0 - |\gamma-\gamma_0|$ and we can eliminate p from the minimisation problem which leads to the unconstrained functional

$$\begin{aligned}
\mathcal{I}_{\boldsymbol{f},\gamma_0,p_0}(\boldsymbol{\phi},\gamma) = \int_\Omega \Big\{ & U(\det \boldsymbol{F}) + \tfrac{\mu}{2}(\operatorname{tr}\boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} + 2\gamma C_{mn} + \gamma^2 C_{mm})\\
& + \tfrac{a}{2}\,(\gamma-\gamma_0)^2 + (r-ap_0)|\gamma-\gamma_0| - \boldsymbol{f}\cdot\boldsymbol{\phi}\Big\}\,\mathrm{d}\boldsymbol{x}.
\end{aligned}$$

To eliminate γ from the minimisation process, we perform a variation of $\mathcal{I}_{\boldsymbol{f},\gamma_0,p_0}$ with respect to γ to see

$$0 \in \mu C_{mn} + \mu\gamma C_{mm} + a(\gamma-\gamma_0) + (r-ap_0)\operatorname{sign}(\gamma-\gamma_0). \tag{6.5}$$

By inspection it can be shown that (6.5) has the unique solution (writing $(\cdot)_+ := \max\{0,\cdot\}$)

$$\gamma \in \gamma_0 - \frac{(\mu|C_{mn}+\gamma_0 C_{mm}| - r + ap_0)_+}{\mu C_{mm} + a}\operatorname{sign}(C_{mn}+\gamma_0 C_{mm}).$$

A substitution into $\overline{\mathcal{I}}_{\boldsymbol{f},\gamma_0,p_0}(\boldsymbol{\phi},\gamma)$ leads to the reduced functional

$$\mathcal{I}^{\mathrm{red}}_{\boldsymbol{f},\gamma_0,p_0}(\boldsymbol{\phi}) = \int_\Omega \left\{ \Psi^{\mathrm{red}}_{\gamma_0,p_0}(\mathrm{D}\boldsymbol{\phi}) - \boldsymbol{f}\cdot\boldsymbol{\phi}\right\}\mathrm{d}\boldsymbol{x}$$

with corresponding reduced density function (where $(\cdot)_+^2$ means $((\cdot)_+)^2$)

$$\Psi^{\mathrm{red}}_{\gamma_0,p_0}(\boldsymbol{F}) = U(\det \boldsymbol{F}) + \frac{\mu}{2}(\operatorname{tr} \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} + 2\gamma_0 C_{mn} + \gamma_0^2 C_{mm}) - \frac{1}{2(\mu C_{mm} + a)}\left(\mu|C_{mn} + \gamma_0 C_{mm}| - r + ap_0\right)_+^2 . \tag{6.6}$$

To investigate the convexity properties of the potential $\Psi^{\mathrm{red}}_{\gamma_0,p_0}$, consider first $\gamma_0 = 0$, $p_0 = 0$, i.e., we look at a time–increment at the beginning of which the body is completely elastic. Let us specify $\boldsymbol{F}$ as

$$\boldsymbol{F} = \mathbf{1} + \frac{\alpha}{2}\,(\boldsymbol{m} + \boldsymbol{n}) \otimes (\boldsymbol{n} - \boldsymbol{m}). \tag{6.7}$$

Note that (6.7) constitutes a rank–one family of matrices parameterised by α; $\boldsymbol{F}$ represents a simple shear under an angle of 45 degrees with respect to the plastic slip–system given. Substitution of (6.7) into $\Psi^{\mathrm{red}}_{\gamma_0,p_0}$ yields

$$\tilde{\Psi}(\alpha) = \mu + \frac{\mu}{2}\,\alpha^2 - \frac{(\frac{\mu}{2}\,\alpha^2 - r)_+^2}{2a + \mu(2 - 2\alpha + \alpha^2)}. \tag{6.8}$$

Since $\tilde{\Psi}(\alpha)$ is continuously differentiable, convexity can be studied by means of the sign of the second derivative. A straightforward calculation yields that $\tilde{\Psi}''(\alpha) \geq 0$ everywhere provided a is large enough. So in this case $\tilde{\Psi}(\alpha)$ is convex. This supports the expectation that the presence of hardening should have a regularising effect on the problem at hand.

Let us now consider the opposite case $a = 0$. Then, for r small enough, $\tilde{\Psi}(\alpha)$ is clearly non–convex. For instance, $\tilde{\Psi}''(\alpha) = \frac{\mu}{2}((\frac{2r}{\mu})^2 - 3) < 0$ for $\alpha = 1 > \frac{2r}{\mu}$. By continuity, this holds if $|\gamma_0|$, $|p_0|$, or a remain small.

Proposition 6.1. *There exist positive constants c_1, c_2, c_3, c_4, such that for all $|\gamma_0| < c_1$, $|p_0| < c_2$, $r < c_3$ and $a < c_4$ the potential $\Psi^{\mathrm{red}}_{\gamma_0,p_0}(\boldsymbol{F})$ given in (6.6) is not rank–one convex.*

This result implies especially that $\Psi^{\mathrm{red}}_{\gamma_0,p_0}(\boldsymbol{F})$ is not quasiconvex and so suggests the occurrence of microstructures as minimisers of energy, see [BaJ87], [BaJ92] for these notions. To illustrate the possibility of microstructures, let us consider the case $\mu = 2$, $a = 0$ and $r = 1$ with $\tilde{\Psi}(\alpha)$ displayed in Figure 1.

It is easy to show that there exist exactly two values α_1, α_2 such that

$$\tilde{\Psi}'(\alpha_1) = \tilde{\Psi}'(\alpha_2) = \frac{\tilde{\Psi}(\alpha_2) - \tilde{\Psi}(\alpha_1)}{\alpha_2 - \alpha_1}.$$

A numerical calculation yields $\alpha_1 = 0.44061$ and $\alpha_2 = 2.53198$. This means there exists a common tangent of the points $(\alpha_1, \tilde{\Psi}(\alpha_1))$ and $(\alpha_2, \tilde{\Psi}(\alpha_2))$ also depicted in Figure 1.

The interpretation is that any macroscopic deformation gradient (6.7) with parameter $\alpha_1 < \alpha < \alpha_2$ yields a microstructure to lower the macroscopic energy from $\tilde{\Psi}(\alpha)$ to the smaller energy described by the tangent in Figure 1. This is achieved by finer and finer layers

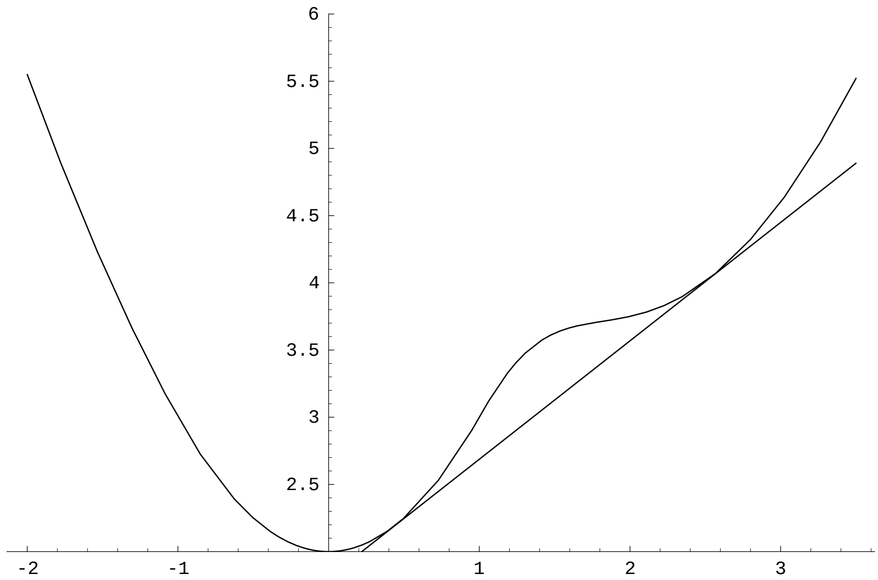

FIGURE 1. $\tilde{\Psi}(\alpha)$ for $\mu = 2$, $a = 0$, $r = 1$

of alternating constant gradients $\mathbf{1}+\frac{\alpha_j}{2}\,(\boldsymbol{m}+\boldsymbol{n})\otimes(\boldsymbol{n}-\boldsymbol{m})$ with probability $|\alpha_j-\alpha|/|\alpha_2-\alpha_1|$. The corresponding microscopic displacement is shown in Figure 2

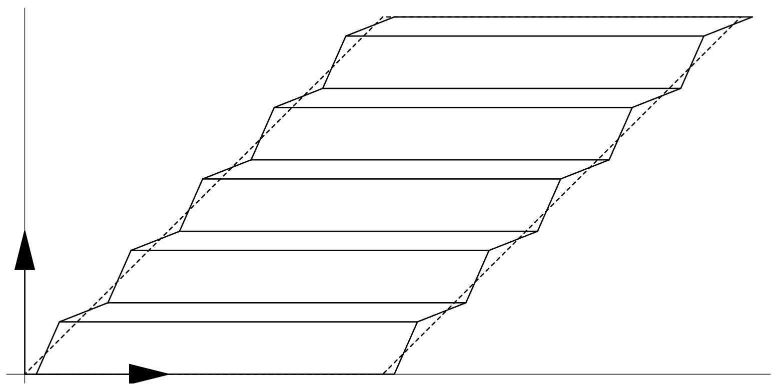

FIGURE 2. Microscopic Displacement for Single Slip–System with Parameter $\alpha_1 < \alpha < \alpha_2$

Remark 6.2 (Infinitesimal elastoplasticity.). In the case of infinitesimal (small–strain) elastoplasticity (6.1) would be replaced by the linear, isotropic energy density function

$$\overline{\Psi}(\boldsymbol{\varepsilon}_{\mathrm{e}}, p) = \frac{\lambda}{2}(\operatorname{tr}\boldsymbol{\varepsilon}_{\mathrm{e}})^2 + \mu \operatorname{tr}\boldsymbol{\varepsilon}_{\mathrm{e}}^2 + \frac{a}{2}\,p^2,$$

where λ, μ are Lamé–parameters and $\boldsymbol{\varepsilon}_{\mathbf{e}}$ denotes elastic strain given by the additive decomposition

$$\boldsymbol{\varepsilon}_{\mathbf{e}} = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\mathbf{p}}.$$

Here $\boldsymbol{\varepsilon}_{\mathbf{p}}$ is the plastic strain and $\boldsymbol{\varepsilon}$ the total strain given by

$$\boldsymbol{\varepsilon} = \operatorname{sym} \boldsymbol{F} - \mathbf{1}.$$

Choosing $\boldsymbol{P} = -\boldsymbol{\varepsilon}_{\mathbf{p}}$ and considering $\boldsymbol{F}_{\mathbf{p}} \approx \mathbf{1}$ for infinitesimal strains we obtain

$$\boldsymbol{Q} = \overline{\boldsymbol{Q}} = \boldsymbol{\sigma},$$

the linearised stress tensor. The flow rule asserts

$$\left(\dot{\boldsymbol{P}}, \dot{p}\right) = \dot{\lambda}\left(\operatorname{sign}(\boldsymbol{m} \cdot \overline{\boldsymbol{Q}}\,\boldsymbol{n}) \operatorname{sym} \boldsymbol{m} \otimes \boldsymbol{n}, -1\right),$$

from which we obtain

$$\boldsymbol{P} = \gamma \operatorname{sym} \boldsymbol{m} \otimes \boldsymbol{n}.$$

The same reasoning as before leads to the internal energy function

$$\Psi^{\mathrm{red}}_{\gamma_0,p_0}(\boldsymbol{F}) = \frac{\lambda}{2}(\operatorname{tr}\boldsymbol{\varepsilon})^2 + \mu \operatorname{tr}\boldsymbol{\varepsilon}^2 + 2\mu\gamma_0\varepsilon_{mn} - \frac{1}{2(\mu+a)}\left(\mu|2\varepsilon_{mn}+\gamma_0| - r + ap_0\right)_+^2, \tag{6.9}$$

with $\varepsilon_{mn} = \boldsymbol{m} \cdot \boldsymbol{\varepsilon}\boldsymbol{n}$.

The density function (6.9) is convex in ($\boldsymbol{\varepsilon}$ and so in) $\boldsymbol{F}$ [ACZ98]. This also indicates that the infinitesimal model is different from that one which may be obtained by expansion of the finite model with respect to small quantities.

7. von Mises plasticity

The von Mises yield–criterion is commonly accepted to model the plastic behaviour of polycristalline metals and other isotropic materials such as various polymers. We consider once again the compressible neo–Hooke material defined by equation (6.1). The yield–function will now be given by

$$\overline{\varphi}(\overline{\boldsymbol{Q}}, q) = |\operatorname{dev}\operatorname{sym}\overline{\boldsymbol{Q}}\,| - r - q. \tag{7.1}$$

Here $\operatorname{dev}\boldsymbol{T} = \boldsymbol{T} - \frac{1}{d}\operatorname{tr}\boldsymbol{T}$ denotes the deviator of a tensor $\boldsymbol{T}$ and $|\boldsymbol{T}\,| = \sqrt{\operatorname{tr}(\boldsymbol{T}^2)}$. We still have $p, q \in \mathbb{R}$, $q \geq 0$. This constitutes the finite strain version of the von Mises yield function with isotropic hardening as derived in [Mie94] or [Hac97]. The flow rule (2.5) can now be put in the form

$$\boldsymbol{P}^{-1}\dot{\boldsymbol{P}} = \dot{\lambda}\operatorname{sign}(\operatorname{dev}\operatorname{sym}\overline{\boldsymbol{Q}}), \qquad \dot{p} = -\dot{\lambda}. \tag{7.2}$$

Here $\operatorname{sign}(\boldsymbol{A}) := \boldsymbol{A}/|\boldsymbol{A}|$ if $\boldsymbol{A} \neq 0$ and $\operatorname{sign}(\mathbf{0})$ constitutes the closed unit ball of matrices intersected with the symmetric, trace–free matrices. Hence $\operatorname{tr}\boldsymbol{P}^{-1}\dot{\boldsymbol{P}} = 0$ which, together with the initial condition $\boldsymbol{P}(0) = \mathbf{1}$, implies $\det\boldsymbol{P} = 1$. Although this relation is not assumed to hold a priori we use it to eliminate $\det\boldsymbol{P}$ from $\overline{W}$ further on.

The corresponding Legendre–transformed potential is (similar to [ACZ98]) given as

$$\begin{aligned} J^*(\boldsymbol{S}, s) &= \sup\left\{ \overline{\boldsymbol{Q}} : \boldsymbol{S} + qs \ : \ |\operatorname{dev}\operatorname{sym}\overline{\boldsymbol{Q}}\,| - q \le r, \quad q \ge 0 \right\} \\ &= \begin{cases} r|\boldsymbol{S}| & \text{if } \operatorname{tr}\boldsymbol{S} = 0,\ \boldsymbol{S} = \boldsymbol{S}^{\mathrm{T}} \text{ and } |\boldsymbol{S}| + s \le 0, \\ \infty & \text{else.} \end{cases} \end{aligned}$$

In this example, the choice of the increment $\Delta(\boldsymbol{P}, \boldsymbol{P}_0)$ of plastic deformation is of particular importance. Volume preservation of plastic flow can either be expressed in direct form as $\det \boldsymbol{P} = 1$ of in rate form as $\operatorname{tr} \boldsymbol{P}^{-1}\dot{\boldsymbol{P}} = 0$. The specific form of the potential J^* implies that the latter condition is carried over to the time–incremental problem as $\operatorname{tr}\Delta(\boldsymbol{P}, \boldsymbol{P}_0) = 0$. This condition, however, does not automatically imply $\det \boldsymbol{P} = 1$ (here von Mises plasticity differs from the model discussed in the previous section), which means we have to construct the time increment $\Delta(\boldsymbol{P}, \boldsymbol{P}_0)$ in such a way as to ensure $\det \boldsymbol{P} = 1$. There is no obvious way to achieve this. One possible solution is

$$\Delta(\boldsymbol{P}, \boldsymbol{P}_0) = \log(\boldsymbol{P}_0^{-1}\boldsymbol{P}). \tag{7.3}$$

For $\boldsymbol{P}_0^{-1}\boldsymbol{P}$ symmetric and positive definite the logarithm is always well defined and can be calculated, e.g., from a singular value decomposition. On the other hand for given symmetric $\boldsymbol{S} = \Delta(\boldsymbol{P}, \boldsymbol{P}_0)$ we have $\boldsymbol{P} = \boldsymbol{P}_0 \exp \boldsymbol{S}$, hence $\det \boldsymbol{P}_0 = 1$ and $\operatorname{tr}\boldsymbol{S} = 0$ imply $\det \boldsymbol{P} = 1$. Numerical time–integration algorithms based on such formulations are quite common in finite–strain elastoplasticity [Mie94, MiS93].

Substitution of the specific forms of J^* and $\Delta(\boldsymbol{P}, \boldsymbol{P}_0)$ leads to the reduced functional

$$\overline{\mathcal{I}}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\boldsymbol{\phi}, \boldsymbol{P}, p) = \int_\Omega \Big\{ U((\det \boldsymbol{C})^{1/2}) + \frac{\mu}{2}\operatorname{tr}(\boldsymbol{P}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{P}) + \frac{a}{2}p^2 + r|\log(\boldsymbol{P}_0^{-1}\boldsymbol{P})| - \boldsymbol{f}\cdot\boldsymbol{\phi} \Big\}\,\mathrm{d}\boldsymbol{x}, \tag{7.4}$$

with the three constraints

$$\operatorname{tr}\log(\boldsymbol{P}_0^{-1}\boldsymbol{P}) = 0, \qquad \boldsymbol{P}_0^{-1}\boldsymbol{P} = (\boldsymbol{P}_0^{-1}\boldsymbol{P})^{\mathrm{T}}, \qquad |\log(\boldsymbol{P}_0^{-1}\boldsymbol{P})| + p - p_0 \le 0.$$

The second and third constraint can be eliminated: Minimising with respect to p gives

$$p = p_0 - |\log(\boldsymbol{P}_0^{-1}\boldsymbol{P})|. \tag{7.5}$$

We introduce the symmetric tensor $\boldsymbol{S}$ as a new independent variable via the substitution $\boldsymbol{P} = \boldsymbol{P}_0 \exp \boldsymbol{S}$. The substitution of (7.5) into (7.4) yields

$$\begin{aligned} \overline{\mathcal{I}}_{\boldsymbol{f},\boldsymbol{P}_0,p_0}(\boldsymbol{\phi}, \boldsymbol{S}, p) = \int_\Omega \Big(U((\det \boldsymbol{C})^{1/2}) + \frac{\mu}{2}\operatorname{tr}\big((\exp \boldsymbol{S})\boldsymbol{P}_0^{\mathrm{T}}\boldsymbol{C}\boldsymbol{P}_0(\exp \boldsymbol{S})\big) + \frac{a}{2}|\boldsymbol{S}|^2 \\ + (r - ap_0)|\boldsymbol{S}| - \boldsymbol{f}\cdot\boldsymbol{\phi}\Big)\,\mathrm{d}\boldsymbol{x} \end{aligned} \tag{7.6}$$

up to a fixed additive constant. There is one remaining constraint

$$\operatorname{tr}\boldsymbol{S} = 0.$$

The reduced internal energy reads

$$\Psi^{\mathrm{red}}_{\boldsymbol{P}_0,p_0}(\boldsymbol{F}) = \inf\Big\{ U((\det \boldsymbol{C})^{1/2}) + \frac{\mu}{2}\,\mathrm{tr}\Big((\exp \boldsymbol{S})\boldsymbol{P}_0^{\mathrm{T}}\boldsymbol{C}\boldsymbol{P}_0(\exp \boldsymbol{S})\Big) + \frac{a}{2}\,|\boldsymbol{S}|^2 + (r - ap_0)|\boldsymbol{S}| \;\Big|\; \boldsymbol{S} = \boldsymbol{S}^{\mathrm{T}},\ \mathrm{tr}\,\boldsymbol{S} = 0 \Big\}. \tag{7.7}$$

There is no analytical expression for $\Psi^{\mathrm{red}}_{\boldsymbol{P}_0,p_0}(\boldsymbol{F})$, but we can still study its convexity properties by performing the minimisation in (7.7) numerically. In order to do this we have to specify the function $U(j)$. A common choice is

$$U(j) = \frac{\lambda}{4} j^2 - \frac{\lambda + 2\mu}{2} \log j. \tag{7.8}$$

We have $U(j) \to \infty$ for $j \to 0$ which prohibits the compression to zero volume with finite force. Also (7.8) reduces to isotropic elastic material in the infinitesimal case with Lamé–parameters λ and μ.

Once again $\Psi^{\mathrm{red}}_{\boldsymbol{P}_0,p_0}$ is not rank–one convex. In order to show this let us define

$$\tilde{\Psi}(\alpha) = \Psi^{\mathrm{red}}_{\mathbf{1},0}(\mathbf{1} + \alpha\,\boldsymbol{n} \otimes \boldsymbol{n}),$$

where $\boldsymbol{n}$ is an arbitrary unit vector. (Because of isotropy of $\Psi^{\mathrm{red}}_{\boldsymbol{P}_0,p_0}$ the definition is independent from the choice of $\boldsymbol{n}$.) Figure 3 shows the graphs of $\tilde{\Psi}(\alpha)$ and $\tilde{\Psi}''(\alpha)$ and a clear indication of non–convex behaviour. (Note that for $\lambda > 0$ but small enough we have $\tilde{\Psi}''(\alpha) > 0$ for large α while $\tilde{\Psi}(\alpha)$ still remains non–convex.)

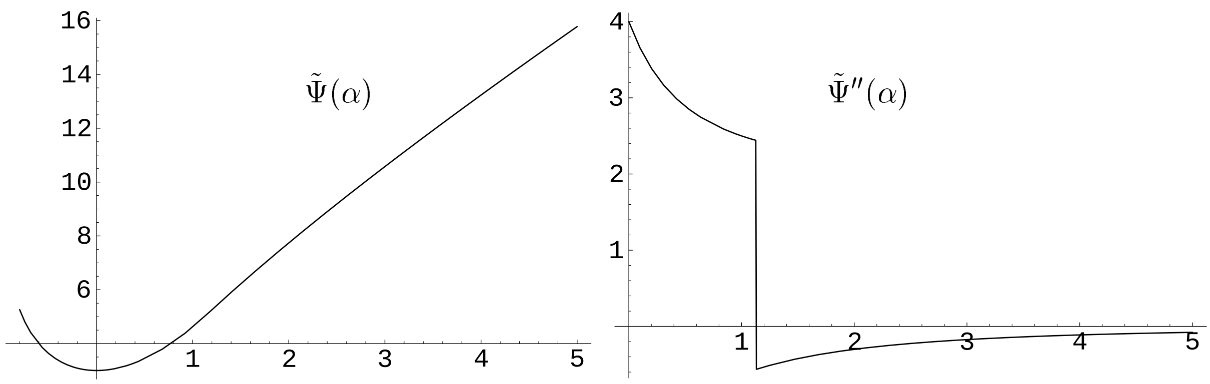

FIGURE 3. $\tilde{\Psi}(\alpha)$, $\tilde{\Psi}''(\alpha)$ for $\lambda = 0$, $\mu = 2$, $a = 1$, $r = 5$

A remarkable feature of this example is that, surprisingly and opposite from what is found in classical elastoplasticity, even a substantial amount of hardening does not prevent the loss of (rank–one) convexity.

Remark 7.1 (Infinitesimal elastoplasticity). In the same way as in Remark 6.2 we can perform the transition to the infinitesimal case. This results in an internal energy

$$\Psi^{\mathrm{red}}_{\boldsymbol{P}_0,p_0}(\boldsymbol{F}) = \frac{\lambda}{2}(\operatorname{tr}\boldsymbol{\varepsilon})^2 + \mu\operatorname{tr}\boldsymbol{\varepsilon}^2 + 2\mu\operatorname{tr}(\boldsymbol{P}_0\boldsymbol{\varepsilon}) - \frac{1}{2(2\mu+a)}\left(2\mu|\operatorname{dev}(\boldsymbol{\varepsilon}+\boldsymbol{P}_0)| - r + ap_0\right)_+^2,$$

which once again turns out to be convex in $\boldsymbol{F}$ [ACZ98]. Consequently, the infinitesimal model differs fundamentally from the finite one.

Appendix A. Discussion and additional mathematical theory

This appendix provides some mathematical concepts employed in the preceding three sections. Besides notions of quasiconvexity [Dac89] we discuss cross–quasiconvexity and motivate the necessity (not only the convenience) of the reduced problem in order to detect microstructure.

Definition A.1 (quasiconvexity). *A function $\psi : \mathbb{R}^{d\times d} \to \mathbb{R}$ is called quasiconvex if it satisfies*

$$\psi(\boldsymbol{F}) \leq \frac{1}{\operatorname{vol}(B)}\int_{\boldsymbol{y}\in B}\psi(\boldsymbol{F}+\mathrm{D}\tilde{\boldsymbol{\phi}}(\boldsymbol{y}))\,\mathrm{d}\boldsymbol{y} \tag{A.1}$$

for all $\tilde{\boldsymbol{\phi}} \in \mathrm{W}^{1,\infty}_0(B,\mathbb{R}^d)$ ($_0$ denotes homogeneous Dirichlet boundary conditions on ∂B).

Here the set $B\subset\mathbb{R}^d$ is any open domain in $\mathbb{R}^d$, however it suffices to consider the unit ball.

It is well established by now that the loss of quasiconvexity gives rise to nonexistence of minimisers and hence to the formation of microstructure in infimising sequences, cf. [BaJ87, BaJ92]. The above examples show that Ψ^{red} is not quasiconvex (indeed not even rank–one convex) for typical examples of finite–strain plasticity. This is to some extent surprising since infinitesimal plasticity is, at least in the presence of hardening, well posed (see Remark 7.1 above). The lack of convexity of the corresponding potentials should coincide with the occurrence of microstructures in the associated material models.

Such microstructures are indeed observed experimentally in form of localisation zones or shear bands, especially in the plasticity of metals or geomaterials, [Kor98, Per98]. They effectively are first–order laminates consisting of alternating bands with high and small or no plastic deformation. Such shear bands usually are attributed to loss of ellipticity of the corresponding model, i.e., the Cauchy–Hadarmard condition is violated (this is equivalent to the loss of rank–one convexity). But even higher–order laminates should be expected. These are generally not attributed to plastic materials, but even here experimental evidence can be found, [Kor98, OrR99].

So far our theoretical findings are in agreement with experimental results. There are, however, new insights to be gained in the field of mechanics of materials as well. Up to now localisation phenomena have always been believed to be associated with the presence of material softening, usually caused by some sort of material damage. Hence any description of shear bands had to involve some sort of damage model or at least some phenomenological softening model. Our results show, that finite–strain plasticity in itself is already capable of exhibiting localisation effects of this kind without invoking any additional models, thus allowing us to explain those phenomena using fewer and maybe better justified constitutive assumptions.

Comments on the associated mathematical structures behind of our theory conclude the appendix. The question we want to follow here is why the reduced incremental minimisation problem (5.2) is more tractable than the full incremental minimisation problem (4.3). The basic source is that all our existence theory of the minimsation problems relies on showing coerciveness and weak lower semicontinuity of the functional on suitable function spaces. However, weak lower semicontinuity is only sufficient but not necessary for the existence of minimisers.

The full functional has the general structure

$$\mathcal{I}(\boldsymbol{\phi}, z) = \int_\Omega \psi(\boldsymbol{x}, \mathrm{D}\boldsymbol{\phi}(\boldsymbol{x}), z(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x} - \ell(\boldsymbol{\phi}), \tag{A.2}$$

where the integral density $\psi : \Omega \times \mathbb{R}^{d\times d} \times \mathbb{R}^k \to \mathbb{R}$ depends only locally on the internal variable $z \in \mathbb{R}^k$ not involving any derivatives. Such a structure occurs in many continuum mechanical problems, such as phase transformations problems, where z describes the volume fractions of the different phases ([MTL00, GoM00], or in shell–models [LDR99]). Up to technical details (like growth conditions and continuity) the weak lower semi–continuity of the functional $\mathcal{I}$ on $\mathrm{W}^{1,q_1}(\Omega, \mathbb{R}^d) \times \mathrm{L}^{q_2}(\Omega, \mathbb{R}^k)$ (with suitable $q_1, q_2 \in (1, \infty)$) is equivalent to the **cross–quasiconvexity**, see [LDR99] and the references therein where also the relation to the more general notion of A–quasiconvexity ([Dac82, FoM99]) is discussed.

Definition A.2 (cross–quasiconvexity). *The function $\psi : \mathbb{R}^{d\times d} \times \mathbb{R}^k \to \mathbb{R}$ is called cross–quasiconvex, if for all $(\boldsymbol{F}^*, z^*) \in \mathbb{R}^{d\times d} \times \mathbb{R}^k$ we have*

$$\psi(\boldsymbol{F}^*, z^*) \le \frac{1}{\mathrm{vol}(B)} \int_{\boldsymbol{y}\in B} \psi(\boldsymbol{F}^* + \mathrm{D}\tilde{\boldsymbol{\phi}}(\boldsymbol{y}), z^* + \tilde{z}(\boldsymbol{y}))\,\mathrm{d}\boldsymbol{y} \tag{A.3}$$

for all $\tilde{\boldsymbol{\phi}} \in \mathrm{W}^{1,\infty}_0(B, \mathbb{R}^d)$ and all $\tilde{z} \in \mathrm{L}^\infty(B, \mathbb{R}^k)$ with $\int_B \tilde{z}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = 0$.

Immediate consequences of cross–quasiconvexity are the quasiconvexity (see (A.1)) of $\psi(\boldsymbol{x}, \cdot, z) : \mathbb{R}^{d\times d} \to \mathbb{R}$ (choose $\tilde{z} \equiv 0$ in (A.3)) and the convexity of $\psi(\boldsymbol{x}, \boldsymbol{F}, \cdot) : \mathbb{R}^k \to \mathbb{R}$ (choose $\tilde{\boldsymbol{\phi}} \equiv 0$ in (A.3)). In general, these two conditions are not sufficient to guarantee cross–quasiconvexity.

The situation in finite plasticity is even worse. We cannot have convexity in the internal variable $z = (\boldsymbol{P}, p)$ as Ψ is defined via (4.2), frame indifference implies non–convexity of $\overline{W}(\cdot, p)$ and the convexity of J^* will not restore convexity of $\boldsymbol{P} \mapsto \Psi(\boldsymbol{F}, \boldsymbol{P}, p; \boldsymbol{P}_0, p_0) = \overline{W}(\boldsymbol{F}\boldsymbol{P}, p) + J^*(\Delta(\boldsymbol{P}_0, \boldsymbol{P}), p - p_0)$.

We are thus forced to study the reduced functional $\mathcal{I}^{\mathrm{red}}$ with the reduced density

$$\psi^{\mathrm{red}}(\boldsymbol{x},\boldsymbol{F}) = \inf\left\{\ \psi(\boldsymbol{x},\boldsymbol{F},z)\ \middle|\ z\in\mathbb{R}^k\ \right\}.$$

Under very weak assumptions (like continuity of $\psi(\boldsymbol{x},\boldsymbol{F},\cdot):\mathbb{R}^k\to\mathbb{R}$ and growth at infinity) we obtain that the infimum in this definition is really a minimum and we may construct a (measurable) map $Z:\Omega\times\mathbb{R}^{d\times d}\to\mathbb{R}^k$ such that $\psi^{\mathrm{red}}(\boldsymbol{x},\boldsymbol{F}) = \psi(\boldsymbol{x},\boldsymbol{F},Z(\boldsymbol{x},\boldsymbol{F}))$. The incremental minimisation problem for $\mathcal{I}$ in (A.2) is solved as soon as we have found the minimiser $\boldsymbol{\phi}$ of the reduced functional $\mathcal{I}^{\mathrm{red}}$ on $\mathrm{W}^{1,p_1}(\Omega,\mathbb{R}^d)$. In fact, we only let $z(x) = Z(x,\mathrm{D}\boldsymbol{\phi}(\boldsymbol{x}))$.

To obtain a minimiser for $\mathcal{I}^{\mathrm{red}}$ it is sufficient to have quasiconvexity of ψ^{red} which is much weaker than cross–quasiconvexity of ψ. In fact, cross–quasiconvexity of ψ immediately implies the quasiconvexity of ψ^{red}. However, the hope for finite elastoplasticity is that under suitable assumptions we may have quasiconvexity of ψ^{red} without cross–quasiconvexity of ψ.

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Max Planck Institut for Mathematics in the Sciences, Inselstr. 22-26, D-04103 Leipzig, Germany. (On Leave from Mathematisches Seminar, Christian-Albrechts-Universität zu Kiel, Germany.)

E-mail address: cc@numerik.uni-kiel.de

Lehrstuhl für Allgemeine Mechanik, Ruhr–Universität Bochum, D–44780 Bochum, Germany.

E-mail address: hackl@am.bi.ruhr-uni-bochum.de

Mathematisches Institut A, Universität Stuttgart, D–70569 Stuttgart, Germany.

E-mail address: mielke@mathematik.uni-stuttgart.de