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A plasticity theory of solids with a macroscopic phase parameter

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Abstract

In the framework of rate-independent finite-strain elasto-plasticity a model is derived that describes plasticity for certain composites undergoing phase transformations under isothermal conditions. We show the thermodynamic validity of the equations. Then the effect of phase transitions is studied and it is demonstrated in two examples that phase transitions oppose to the generation of microstructure. In particular, we show that there is no microstructure in the region of the slip band where the bulk phase has just formed.

1. Introduction

This article deals with phase transitions and the formation of microstructure in solids that undergo plastic deformations, possibly accompanied by diffusion, under isothermal conditions.

There exists already rich literature on the mechanics of such systems. Beginning with the pioneering work of Ericksen, [14], where phase transitions in a one-dimensional bar induced by shear were studied, the problem was investigated further by many authors. Here we only mention [22], [1], [18], [38] and [32]. Also, there has been intense studies on selected material systems, in particular on steels, e.g. [16], [17], [12], [11] and [19], which contributed significantly to the common understanding of the involved mechanical concepts.

In contrast to the existing work, in the approach presented here the stored mechanical energy W depends additionally on a phase parameter χ that accounts for macroscopic changes in the structure of the material. As explicit application we have in mind the class of metallic-intermetallic laminates (MIL), see for instance [36], [37]. MIL materials form a special class of composites where elements of macroscopic size ($\approx 1mm$) of two or more different metals are combined to enhance the mechanical, electrical or magnetic properties of the individual species.

The introduction of a macroscopic phase variable χ in our model allows in a natural way to incorporate the surface energy between the blocks of the composite. Furthermore, this allows for a clear separation of the spatial variations on the macroscopic scale, i.e. the variation of χ, and of the variations of the microstructure on a small length scale.

Different to the earlier work [5], where diffusional reconstitutive phase transitions are investigated and the influence of the generation of vacancies to the diffusion concentration and the shape of the interface is studied, the plastic behaviour of the material is modelled here within the framework of rate-independent finite-strain elasto-plasticity that goes back to Hill, [20], and Rice, [34]. We use rate-independent finite-strain elastoplasticity in this article, as it implies plastic response by the material only under certain conditions and may otherwise lead to a purely elastic behaviour. Thus, in contrast to rate-dependent formulations, the plastic slip systems are not permanently active. This simplifies our analysis in the sections 4 and 5. Nevertheless, as is well known, the rate-independent theory has the possible drawback that for non-convex settings, the uniqueness of the mechanical solution may get lost.

Further key to the mathematical formulation is the minimum formulation (21) of the free energy. The idea of incorporating diffusion by imposing a corresponding constraint on the minimisation of the free energy functional was used before in [2].

The analysis is based on three key assumptions. The first is that the minimum of the free energy is attained, i.e. that during the time-evolution the system does not stop before a minimum is reached. The second assumption is that the principle of maximal plastic dissipation holds, which gives rise to the flow rule (7). Finally, we assume that the yield function Y does not depend on the plastic deformation. For general materials, all these assumptions can be violated.

In [9], a unifying theory for the relative motion of crystal grains is developed, including sliding, rotation, shrinking and mechanical twinning. We want to point out that our ansatz for the yield function, (38) and (31), especially the spatial localisation expressed by introducing the set S, can be subsumed below this theory.

This article is organised in the following way. In Section 2 we derive the mathematical formulation. Section 3 discusses the Euler-Lagrange equations valid for minimisers of the free energy and shows the correctness of the approach. Also, the second law of thermodynamics is validated. In Section 4 we discuss a single slip system and analyse the consequences of phase transitions to the model in this case. In Section 5 the case of von Mises plasticity is analysed. Also, the effect of diffusion is studied numerically. As main result of these two sections, it is shown that in the 'flip set', that is the set where the phase parameter has recently changed, the free energy functional is convex implying the absence of any microstructure.

2. Derivation of the model

We consider a two-phase segregation problem under isothermal conditions with constant temperature θ. The crystal is described by a reference domain $\Omega \subset \mathbb{R}^3$, where Ω is a bounded domain with Lipschitz boundary. In order to keep track of the deformations, for fixed stop time $\mathcal{T} > 0$ we introduce the mapping

$$\varphi : \Omega \times [0, \mathcal{T}] \to \Omega_t,$$

with $\Omega_t := \{\varphi(x,t) \,|\, x \in \Omega\}$ the deformed domain at time $t \in [0, \mathcal{T}]$. The mapping φ is a diffeomorphism of Ω to Ω_t for any $0 \le t \le \mathcal{T}$. Assuming that Ω refers to the undeformed crystal at time $t = 0$, we have $x \mapsto \varphi(x, 0) = \mathrm{Id}$ and $\det D\varphi(x,t) > 0$.

We introduce a phase parameter χ within the functions of bounded variation in Ω. For simplicity we will restrict in this paper to the situation that phases of at most two different types coexist. For $t \in [0, \mathcal{T}]$, let $\chi \in BV(\Omega; \{0,1\})$ be the indicator function of one a-priori chosen phase. For convenience we set $\chi_1 := \chi$ and $\chi_2 := 1 - \chi$.

Let $\mathcal{M} := \mathbb{R}^{3\times 3}$. We define the two matrix groups

$$\begin{aligned} GL_+(\mathbb{R}^3) &:= \Big\{ F \in \mathcal{M} \,\Big|\, \det F > 0 \Big\}, \\ SO(\mathbb{R}^3) &:= \Big\{ R \in \mathcal{M} \,\Big|\, \det R > 0,\ R^t R = 1 \Big\}. \end{aligned}$$

The transformation $F := D\varphi$ is multiplicatively decomposed by

$$F = F_{\mathrm{e}} F_{\mathrm{p}}, \tag{1}$$

splitting F into an elastic part F_{e} and a plastic part F_{p}, with $F_{\mathrm{e}}, F_{\mathrm{p}} \in GL(\mathbb{R}^3)_+$. The decomposition (1) is unique only up to rigid displacements as $F = (F_{\mathrm{e}} \circ R)(R^T \circ F_{\mathrm{p}})$ holds for all $R \in SO(\mathbb{R}^3)$. However, the theory that will be developed depends only on $F_{\mathrm{e}} F_{\mathrm{e}}^t$ and $F_{\mathrm{p}} F_{\mathrm{p}}^t$ which are invariant under rigid rotations R.

In the sequel we will use the plastic variables (P, κ) where $\kappa \in L^2(\Omega; \mathbb{R}^l)$ is an internal variable that describes hardening and $P := F_{\mathrm{p}}^{-1}$. The last definition implies $F_{\mathrm{e}} = D\varphi P$. For simplicity we set $l = 1$ and consider only scalar hardening.

We assume that the mechanical energy depends only on the elastic part of the deformation gradient. This is motivated by the understanding that plastic deformations go along with configurational changes of the material body which do not affect the elastic deformation. A plastic deformation only changes the reference configuration of the body.

Consequently we write the internal mechanical stored energy in the form

$$W(\chi, \kappa, F, F_{\rm p}) = \overline{W}(\chi, \kappa, F F_{\rm p}^{-1}) \tag{2}$$

for a suitable function $\overline{W}$. By frame indifference, $\overline{W}$ must be independent under rigid rotations,

$$\overline{W}(\chi, \kappa, R F F_{\rm p}^{-1}) = \overline{W}(\chi, \kappa, F F_{\rm p}^{-1}) \qquad \text{for all } R \in SO(\mathbb{R}^3).$$

This implies that $\overline{W}$ depends only on the symmetric part $(F_{\rm e}^t F_{\rm e})^{\frac{1}{2}}$ of $F_{\rm e}$ or equivalently only on the nonlinear elastic strain $\varepsilon_e = \frac{1}{2}(F_{\rm e}^t F_{\rm e} - {\rm Id})$.

One example for W corresponds to the class of Neo-Hookean materials, see [13], [29], and in the presence of phase transitions we make the ansatz

$$\overline{W}(\chi, \kappa, F_{\rm e}) := \frac{\nu(\chi)}{2}\|F_{\rm e}\|^2 + \frac{\lambda}{2}|\kappa|^2 + U(\det F_{\rm e}), \tag{3}$$

for given Lamé parameter $\nu > 0$ that depends on the phase χ and hardening parameter $\lambda > 0$. In (3) we set $\|F_{\rm e}\| := \sqrt{{\rm tr}(F_{\rm e}^t F_{\rm e})}$, where ${\rm tr}(A) = \sum_i A_{ii}$ is the trace of a matrix A. The function $U : \mathbb{R}^+ \to \mathbb{R}$ is convex and satisfies $U(d) \to \infty$ for $d \to 0$ and for $d \to \infty$. The minimisation of $\overline{W}$ thus prevents $\det F_{\rm e}$ from becoming singular and prohibits the compression to zero volume with finite energy.

Ansatz (3) represents a macroscopic theory and is convex in $F_{\rm e}$. It is for instance well-suited to model damage in composites, like the recently-discovered intermetallic-metal laminate composites, [36]. Instead of (3) we may choose

$$\overline{W}(\chi, \kappa, F_{\rm e}) := \frac{\nu}{2}\Big[\chi\, {\rm tr}(F_{\rm e}^t F_{\rm e} - M_1) + (1-\chi){\rm tr}(F_{\rm e}^t F_{\rm e} - M_2)\Big] + \frac{\lambda}{2}|\kappa|^2 + U(\det F_{\rm e}), \tag{4}$$

for given symmetric and positive definite deformations M_1, $M_2 \in SO(\mathbb{R}^3)$. This leads to a general model for plasticity in a two-phase material. Both (3) and (4) give rise to a coercive, lower semi-continuous free-energy functional which guarantees the existence of a minimiser, but due to the non-convexity of Ansatz (4) in $F_{\rm e}$, the uniqueness of a minimising $F_{\rm e}$ in the latter case is in general not given.

For given W we now introduce the following thermodynamically conjugate variables. Let the phase modulus ξ, the hardening modulus π, the first Piola-Kirchhoff stress T and the back-stress or Eshelby tensor X that models kinetic hardening be given by

$$\xi = -\frac{\partial W}{\partial \chi}, \quad \pi = -\frac{\partial W}{\partial \kappa}, \quad T = \frac{\partial W}{\partial F}, \quad X = -\frac{\partial W}{\partial P}.$$

The introduction of the minus signs in the definition of π and X has historical reasons. In the considered physical framework it holds $\pi \geq 0$. The variation of $\overline{W}$ with respect to χ is to be understood in the sense

$$\xi = -\overline{W}(\chi = 1, \kappa, F_{\rm e}) + \overline{W}(\chi = 0, \kappa, F_{\rm e}).$$

In the mathematical and physical literature, plastic deformations are usually described by flow rules. Subsequently we will discuss the mathematical framework and will show that these formulations are equivalent to a pointwise free energy minimisation algorithm.

In the sequel we generalise a dual formalism that goes back to [27], where the plastic behaviour of solids without phase changes and diffusion is studied. We shall define the yield function in such a way that $Y = 0$ may only occur close to the interfacial region.

In order to characterise the time evolution of the inner variables (χ, κ, P), a yield function Y is introduced. It is postulated that Y does not depend on the plastic deformation F_{p}. Since the back stress $\overline{X} := P^t X = -F_{\mathrm{e}}^t \partial_{F_{\mathrm{e}}} \overline{W}(\chi, \kappa, F_{\mathrm{e}})$ is invariant with respect to all plastic deformations, we thus consider yield functions of the form

$$Y_{x,D\chi} = Y_{x,D\chi}(\xi, \pi, \overline{X}).$$

The additional parameters x and $D\chi$ are needed as we want to restrict plasticity to a small region around $\mathrm{supp} D\chi$, see the definition (10) below and the corresponding explanations.

The set of admissible states is specified by

$$\mathit{\Gamma}_{x,D\chi} := \Big\{ (\xi, \pi, \overline{X}) \in \mathbb{R} \times \mathbb{R} \times \mathcal{M} \,\Big|\, Y_{x,D\chi}(\xi, \pi, \overline{X}) \leq 0 \Big\}.$$

We assume that $\mathit{\Gamma}_{x,D\chi}$ is convex and contains $(0, 0, 0)$.

The plastic flow is determined under the assumption that the principle of maximal plastic dissipation, see [35], holds. The Kuhn-Tucker optimality conditions, first used in this context by Moreau, [27], state that the principle can be written as the *flow rule*

$$(\partial_t \chi, \partial_t \kappa, P^{-1} \partial_t P) = \partial_t \mathit{\Lambda} \left(\frac{\partial Y_{x,D\chi}}{\partial \xi}, \frac{\partial Y_{x,D\chi}}{\partial \pi}, \frac{\partial Y_{x,D\chi}}{\partial \overline{X}} \right) \tag{5}$$

for $Y_{x,D\chi}(\xi, \pi, \overline{X}) \leq 0$ and $Y_{x,D\chi}(\xi, \pi, \overline{X}) \partial_t \mathit{\Lambda} = 0$ with Lagrange multiplier $\partial_t \mathit{\Lambda} \geq 0$.

As χ only attains the two discrete values 0 and 1, Equality (5) must be interpreted in the sense of measures: For the validity of the first component of the flow rule, it has to hold for almost all $x \in \mathit{\Omega}$

$$\int_0^T \chi(x, \cdot) \partial_t g \, \mathrm{d}t = \int_0^T \mathit{\Lambda} \frac{\partial Y_{x,D\chi}}{\partial \xi} \partial_t g \, \mathrm{d}t \qquad \text{for all } g \in C_0^\infty(0, T).$$

By Riesz' representation theorem, this relationship defines an identity between the two Borel measures $\partial_t \chi$ and $\partial_t \mathit{\Lambda}$.

For the further understanding of (5) it is important to observe that this approach specifies a non-diffusive flow in χ. The change in χ goes along with a change in plasticity. Equation (5) does not specify an equation of phase-field type in χ.

We define the plastic potential by

$$Q_{x,D\chi}(\xi,\pi,\overline{X}) := \begin{cases} 0 & \text{for } Y_{x,D\chi}(\xi,\pi,\overline{X}) \le 0, \\ \infty & \text{else} \end{cases}$$

and introduce for later use the Fenchel conjugate $Q^\star_{x,D\chi}$ of $Q_{x,D\chi}$ by

$$\begin{aligned} Q^\star_{x,D\chi}(\chi,\kappa,P) &:= \sup_{(\xi,\pi,\overline{X})} \Big\{ \xi\chi + \pi\kappa + \overline{X} : P - Q_{x,D\chi}(\xi,\pi,\overline{X}) \Big\} \\ &= \sup_{(\xi,\pi,\overline{X})\in\Gamma_{x,D\chi}} \Big\{ \xi\chi + \pi\kappa + \overline{X} : P \Big\}. \end{aligned} \tag{6}$$

Using duality theory the rule (5) can be recast to the following condition: *The triple $(\xi,\pi,\overline{X})$ is admissible and maximises the plastic dissipation*

$$\begin{aligned} &-\partial_\chi W(\chi,\kappa,F,P)\partial_t\chi - \partial_\kappa W(\chi,\kappa,F,P)\partial_t\kappa - \partial_P W(\chi,\kappa,F,P) : \partial_t P \\ &\quad = \xi\partial_t\chi + \pi\partial_t\kappa + X : \partial_t P \\ &\quad = \xi\partial_t\chi + \pi\partial_t\kappa + \overline{X} : (P^{-1}\partial_t P). \end{aligned}$$

In other words,

$$\begin{aligned} \xi\partial_t\chi + \pi\partial_t\kappa + \overline{X} : (P^{-1}\partial_t P) \ge{}& s_1\partial_t\chi + s_2\partial_t\kappa \\ &+ S : (P^{-1}\partial_t P) \quad \forall (s_1,s_2,S) \in \Gamma_{x,D\chi}. \end{aligned}$$

By the definition of the subdifferential, this is equivalent to

$$(\partial_t\chi, \partial_t\kappa, P^{-1}\partial_t P) \in \partial^{\text{sub}} Q_{x,D\chi}(\xi,\pi,\overline{X}). \tag{7}$$

Here, $\partial^{\text{sub}} Q_{x,D\chi}$ denotes the subdifferential of $Q_{x,D\chi}$.

We want to derive a variational formulation. To this end it is necessary to pass to the time-discrete setting. The following method goes back to [33]. For small fixed parameter $h > 0$ let $\partial_t^h\kappa(\cdot,t) := (\kappa(\cdot,t) - \kappa(\cdot,t-h))h^{-1}$ approximate $\partial_t\kappa(\cdot,t)$ with the analogous definition of $\partial_t^h\chi(\cdot,t)$. Finally, by $d_t^h(P)$ we denote an approximation of $P^{-1}\partial_t P$.

With this definition, in the time-discrete setting, (7) becomes

$$h(\partial_t^h\chi, \partial_t^h\kappa, d_t^h(P)) \in \partial^{\text{sub}} Q_{x,D\chi(t-h)}(\xi,\pi,\overline{X}) \tag{8}$$

which has to hold for all $x \in \Omega$.

The following Lemma (with straightforward changes due to the additional dependence of $\overline{W}$ on χ) is taken from [10].

Lemma 1 *The property (8) is a consequence of the energy minimisation*

$$\mathcal{I}(\varphi) = \min_{\chi,\kappa,P} \int_\Omega \Big(\overline{W}(\chi,\kappa,D\varphi P) + hQ^\star_{x,D\chi(t-h)}(\partial_t^h\chi, \partial_t^h\kappa, d_t^h(P)) \Big), \tag{9}$$

where the Fenchel conjugate $Q^\star_{x,D\chi}$ is given by (6).

Proof. We rewrite the integrand $Q^*(\partial_t^h\chi, \partial_t^h\kappa, d_t^h(P))$ in (9) and consider

$$\hat{I}(\varphi,\chi,\xi,\kappa,\pi,P,\overline{X}) := \int_\Omega \overline{W}(\chi,\kappa,D\varphi P) + (\chi-\chi^0)\xi + (\kappa-\kappa^0)\pi \\ + h d_t^h(P) : \overline{X} - hQ^*(\xi,\pi,\overline{X})\,dx.$$

The variation of $\hat{I}$ with respect to ξ, π and $\overline{X}$ gives the flow rule (8). The argument is carried out in detail in Section 3. □

For illustration, we introduce a first typical example, the von Mises yield condition, which is discussed in Section 5. This condition reads

$$Y_{x,D\chi}(\xi,\pi,\overline{X}) := \|\mathrm{dev}\ \mathrm{sym}\overline{X}\| - \sigma_Y - \pi + |\xi|\mathcal{X}_{S(D\chi)}. \tag{10}$$

Here, the positive scalar σ_Y is the yield stress. For a measurable set $E \subset \Omega$,

$$\mathcal{X}_E(x) := \begin{cases} 1 & \text{if } x \in E, \\ 0 & \text{otherwise} \end{cases}$$

denotes the characteristic function of E. Plastic slip occurs localised in designated regions of Ω, the *slip bands* $S(D\chi)$. The explicit form of $S(D\chi)$ does not matter for our analysis and depends on the studied material. If the plastic slip occurs within the grains, we may set

$$S(D\chi) := \{x \in \Omega \mid \mathrm{dist}(x, \mathrm{supp} D\chi) \geq \eta\}$$

with a material-dependent parameter $\eta > 0$. For certain ceramic systems however, the designated areas of plasticity are located in a neighbourhood around the interfacial regions and the above definition must be set accordingly.

By Ansatz (10), phase transitions weaken the material whereas hardening, stated here as a linear law, opposes to it.

Beside the mechanical changes, also the mass diffusion can be cast into the framework of free energy minimisation. Let the solid contain $m \geq 1$ different chemical constituents. In order to measure the density of species i, $1 \leq i \leq m$, we introduce functions $\varrho_i : \Omega \times [0,\mathcal{T}] \to \mathbb{R}_{\geq 0}$ and a vacancy density $\varrho_0 : \Omega \times [0,\mathcal{T}] \to \mathbb{R}_{\geq 0}$. Let $\varrho := (\varrho_0,\ldots,\varrho_m)$. Conservation of mass yields

$$\int_\Omega \sum_{i=0}^m \varrho_i(x,t)\,\mathrm{d}x = \int_\Omega 1\,\mathrm{d}x,$$

so the density vector lies in the simplex

$$\Sigma := \left\{ \varrho' = (\varrho_0',\ldots,\varrho_m') \in \mathbb{R}_{\geq 0}^{m+1} \,\middle|\, \sum_{i=0}^m \varrho_i' = 1 \right\}.$$

The free energy Ψ of the system is introduced by

$$\Psi(\mu,\chi,\kappa,\varphi,P)(t) := \int_\Omega |D\chi| + \overline{W}(\chi,\kappa,D\varphi P) + \psi^\star(\mu,\chi) + hQ^\star_{x,D\chi(t-h)}(\partial_t^h\chi,\partial_t^h\kappa,d_t^h(P))\,\mathrm{d}x. \tag{11}$$

In (11), we introduced the Legendre-Fenchel transform of the free energy density $\psi_k(\varrho)$ of phase k by

$$\psi^\star(\mu,\chi) = \sum_{k=1}^2 \chi_k\psi_k^\star(\mu),$$
$$\psi_k^\star(\mu) := \sup_{\varrho\in\mathrm{dom}(\psi_k)} \{\varrho\cdot\mu - \psi_k(\varrho)\}.$$

Furthermore, $\int_\Omega |D\chi| = \|\chi\|_{BV(\Omega)}$, and the interfacial surface energy is normalised to 1, leading to an isotropic surface energy. For the well-definedness of Ψ at $t=0$, we assume that initial values χ_0, κ_0, P_0 are given in Ω together with $\varphi(t=0)=\mathrm{Id}$.

The term $hQ^\star_{x,D\chi(t-h)}(\partial_t^h\chi,\partial_t^h\kappa,d_t^h(P))$ can be interpreted as the energy release larger than the invested elastic energy in the time interval $(t-h,t]$ due to configurational changes.

A possible ansatz for ψ_k is

$$\psi_k(\varrho) := k_B\theta\sum_{i=0}^m \varrho_i\Big(\ln\varrho_i + \frac{E_i^k}{k_B\theta}\Big). \tag{12}$$

Here, k_B is the Boltzmann constant, E_i^k are enthalpic terms. From (12) we directly compute

$$\psi_k^\star(\mu) = k_B\theta e^{-1}\sum_{i=0}^m \exp\Big(\frac{\mu_i - E_i^k}{k_B\theta}\Big). \tag{13}$$

In particular, $\psi_k^\star(\mu)\ge 0$.

The entry μ_i of the vector of chemical potentials $\mu=(\mu_0,\ldots,\mu_m)$ is related to ϱ by

$$\mu_i = \sum_{k=1}^2 \chi_k\frac{\partial\psi_k}{\partial\varrho_i}(\varrho), \quad 0\le i\le m. \tag{14}$$

Plugging in the definition (12) we find

$$\varrho_i = e^{-1}\exp\Big(\frac{\mu_i - E_i^\chi}{k_B\theta}\Big), \tag{15}$$

where $E_i^\chi = \chi E_i^1 + (1-\chi)E_i^2$.

Onsager's law, [30], [31], postulates that every thermodynamic flux is linearly related to every thermodynamic force. Since in our case the thermodynamic forces are the negative chemical potential gradients, we obtain the phenomenological equations, see [23], p.137,

$$J_i = -\sum_{j=0}^{m} L_{ij} \nabla \mu_j, \quad 0 \le i \le m, \tag{16}$$

with a mobility matrix $L \in \mathbb{R}^{(m+1)\times(m+1)}$ which for simplicity we assume to have constant coefficients. The Onsager reciprocity law, [30], [31], [23], states that L has to be symmetric which we assume from now on. Additionally, L is positive semi-definite with one-dimensional kernel.

Let $\tilde{\varrho}_i : \Omega_t \to [0,1]$ be defined by $\tilde{\varrho}_i := \varrho_i \circ \varphi^{-1}$. The conservation of mass yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} m_i(t) &= \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_t} \tilde{\varrho}_i(x,t)\,\mathrm{d}x = \int_{\Omega} \frac{\mathrm{d}}{\mathrm{d}t}\Big[\tilde{\varrho}_i(\varphi(x,t),t)\det D\varphi(x,t)\Big]\,\mathrm{d}x \\ &= \int_{\Omega} \Big(\partial_t \varrho_i(x,t)\det D\varphi(x,t) + \varrho_i(x,t)\partial_t(\det D\varphi(x,t))\Big)\,\mathrm{d}x. \end{aligned} \tag{17}$$

We compute for $X, H \in \mathrm{GL}(\mathbb{R}^3)$ the Fréchet derivative $D(\det(X))H = \det(X)(\mathrm{X}^{-1}\mathrm{H})$. Consequently,

$$\partial_t(\det D\varphi(x,t)) = \det D\varphi(x,t)\mathrm{tr}[\partial_t D\varphi(x,t) D\varphi^{-1}(\varphi(x,t),t)]. \tag{18}$$

Using this result we obtain

$$\begin{aligned} &\int_{\Omega} \varrho_i(x,t)\partial_t(\det D\varphi(x,t))\,\mathrm{d}x \\ &\qquad = \int_{\Omega_t} \varrho_i(\varphi^{-1}(x,t),t)\mathrm{tr}\Big[\partial_t D\varphi(\varphi^{-1}(x,t),t) D\varphi^{-1}(x,t)\Big]\,\mathrm{d}x \\ &\qquad = \int_{\Omega_t} \varrho_i(\varphi^{-1}(x,t),t)\mathrm{tr}[D(\partial_t\varphi(\varphi^{-1}(x,t),t))]\,\mathrm{d}x \qquad (19) \\ &\qquad = \int_{\Omega} \varrho_i(x,t)\mathrm{div}(\partial_t\varphi(x,t))\det D\varphi(x,t)\,\mathrm{d}x. \qquad (20) \end{aligned}$$

From (17) and (19) we obtain the natural formulation for the conservation of mass in Ω_t

$$\partial_t\tilde{\varrho}(x,t) = -\mathrm{div}[J(x,t)+M(x,t)] := \mathrm{div}[L\nabla\mu(x,t) - \tilde{\varrho}(x,t)\partial_t\varphi(\varphi^{-1}(x,t),t)],$$

where the mechanical mass flux is given by $M(x,t) := \tilde{\varrho}(x,t)\partial_t\varphi(\varphi^{-1}(x,t),t)$. Similarly, with (20), the conservation of mass in the variable ϱ reads

$$\partial_t\varrho_i(x,t) + \varrho_i(x,t)\mathrm{div}(\partial_t\varphi(x,t)) = \mathrm{div}(L\nabla\mu(x,t))_i \qquad \text{in } \Omega.$$

Let the time step $h > 0$ be chosen such that $\mathcal{T} = Lh$ for $L \in \mathbb{N}$ and set $t_j := jh$ for $0 \le j \le L$.

In continuation of (9), the evolution of the problem is determined by iteratively solving for $1 \le j \le L$ the time-discrete minimisation problem

$$\Psi(\mu^j, \chi^j, \kappa^j, \varphi^j, F_{\mathrm{p}}^j) \to \min, \tag{21}$$

where the minimum is sought in the spaces

$$\begin{aligned} &\mu^j \in W^{1,2}(\Omega; \mathbb{R}^{m+1}), \quad \chi^j \in BV(\Omega; \{0,1\}), \\ &\kappa^j \in L^2(\Omega; \mathbb{R}), \quad F_{\mathrm{p}}^j \in L^2(\Omega; \mathcal{M}), \\ &\varphi^j \in \Big\{ \Phi \in W^{1,3+\delta}(\Omega; \mathbb{R}^3) \,\Big|\, \Phi(\Omega) = \Omega_{t_j}, \exists \Phi^{-1} \in W^{1,3+\delta}(\Omega_{t_j}; \mathbb{R}^3), \\ &\qquad\qquad \det(D\Phi) > 0 \text{ almost everywhere in } \Omega \Big\} \end{aligned} \tag{22}$$

(with $\delta > 0$ an arbitrary constant and $\mathcal{M}$ the space of real 3×3-matrices) subject to the constraint

$$\int_\Omega \varrho^j = \int_\Omega \varrho^{j-1} + h\mathrm{div}(L\nabla\mu^j) - \varrho^j \mathrm{div}(\varphi^j - \varphi^{j-1}),$$

which we rewrite with (15) in a condition for μ^j (where $F^j = D\varphi^j$)

$$\begin{aligned} \int_\Omega \exp\Big(\frac{\mu^j - E^\chi}{k_B\theta}\Big)\Big(1 + \mathrm{tr}(F^j - F^{j-1})\Big) - he\,\mathrm{div}(L\nabla\mu^j)\,dx \\ = \int_\Omega \exp\Big(\frac{\mu^{j-1} - E^\chi}{k_B\theta}\Big)\,dx \end{aligned} \tag{23}$$

subject to the boundary conditions

$$\mu^j = \overline{\mu}, \quad \partial_{\boldsymbol{n}}\chi^j = 0, \quad \varphi = \overline{\varphi}, \qquad \text{on } \partial\Omega \tag{24}$$

and with the initial conditions (for $j = 0$)

$$\mu^0 = \mu_0, \quad \chi^0 = \chi_0, \quad \kappa^0 = \kappa_0, \quad F_{\mathrm{p}}(\cdot, 0) = 0, \quad \varphi(\cdot, 0) = \mathrm{Id}. \tag{25}$$

In (24), $\boldsymbol{n}$ is the outer normal to $\partial\Omega$ and $\overline{\mu}$, $\overline{\varphi}$ are prescribed values at the domain boundary. Instead of prescribing the deformations $\overline{\varphi}$, one could prescribe the tractions.

Equation (23) supplies us with a constraint on μ^j since with the computation of μ^j, χ^j at time step j, the density $\varrho^j \in \Sigma$ is obtained implicitly from (14) as ψ_1, ψ_2 are convex functions.

In this article we are not going to address the deep question of the time-continuous limit $h \searrow 0$ in (21). In particular it must be clarified whether the spaces (22) are sufficient for the existence theory. We refer the interested reader to [26] and [15] and references therein for the case without phase transitions and without diffusion.

3. Validation of the model

In this section we discuss consequences of (21), (23) and (11) and demonstrate that the chosen ansatz is meaningful. The discussion can be simplified when resolving the Fenchel duals in the Definition (11) and replacing Ψ in (21) by

$$\begin{aligned}
&\tilde{\Psi}(\varrho, \mu, \lambda_1, \xi, \chi, \pi, \kappa, \varphi, \overline{X}, P)(t_j) \\
&:= \int_{\Omega} \Big\{ |D\chi| + \mu \cdot \varrho - \sum_{k=1}^{2} \chi_k \psi_k(\varrho) + \overline{W}(\chi, \kappa, D\varphi P) \\
&\qquad + \lambda_1 \Big[\exp\Big(\frac{\mu - E^\chi}{k_B \theta} \Big) \Big(1 + \operatorname{tr}\big(D\varphi - D\varphi^{j-1} \big) \Big) \\
&\qquad\qquad - he \operatorname{div}(L \nabla \mu) - \exp\Big(\frac{\mu^{j-1} - E^\chi}{k_B \theta} \Big) \Big] \\
&\qquad + h\partial_t^h \chi \xi + h \partial_t^h \kappa \pi + h d_t^h(P) : \overline{X} - Q_{x, D\chi(t_{j-1})}(\xi, \pi, \overline{X}) \Big\} \,\mathrm{d}x.
\end{aligned}$$

The functional $\tilde{\Psi}$ is maximised with respect to ϱ, ξ, π and $\overline{X}$ and minimised with respect to the variables P, χ, κ, φ and μ. The constrained minimisation of Ψ subject to (23) has been replaced by the unconstrained minimisation of $\tilde{\Psi}$ adding a Lagrange multiplier $\lambda_1 \in \mathbb{R}$.

From the stationarity of $\tilde{\Psi}$ with respect to ϱ_i, $0 \leq i \leq m$, we get back (14). The variation with respect to the dual variables $(\xi, \pi, \overline{X})$ yields the flow rule (8).

From the stationarity of $\tilde{\Psi}$ when restricting to smooth transformations of $\{x \in \Omega \,|\, \chi(x,t) = 1\}$ we get back the definition of ξ as well as the Gibbs-Thomson law

$$H = \psi_1(\varrho) - \psi_2(\varrho) \tag{26}$$

that relates the jump of the free energy density $\psi_1(\varrho) - \psi_2(\varrho)$ across the phase boundary to the mean curvature H of the interface. In summary, we see that the shape of the interface is determined by the Gibbs-Thomson law (26), whereas the flow of χ at the interface is determined by (5).

The derivative of $\tilde{\Psi}$ with respect to λ_1 gives back the constraint (23). Computing the variation of $\tilde{\Psi}$ with respect to μ yields $\int_\Omega \varrho = 0$ implying that during the repeated minimisation rule (21) no stationary points of Ψ with regard to μ are reached.

The stationarity of $\tilde{\Psi}$ with respect to φ yields in the absense of volumetric forces after partial integration the standard equilibrium condition

$$\operatorname{div}(T) = 0 \qquad \text{in } \Omega. \tag{27}$$

From the stationarity of $\tilde{\Psi}$ with respect to κ the definition $\pi = -\frac{\partial W}{\partial \kappa}$ in Ω is recovered.

If we choose for example $d_t^h(P(t)) := P(t-h)^{-1} P(t) - \mathrm{Id}$, the variation of $\tilde{\Psi}$ with respect to P gives us

$$-F^t \partial_{F_\mathrm{e}} \overline{W}(\chi, \kappa, F_\mathrm{e}) = (P(t_{j-1})^{-1})^t \overline{X}, \tag{28}$$

which is an approximation of the constitutive law for $\overline{X}$.

In the rest of this section we sketch the validation of the second law of thermodynamics for the equations (21), (23). In the isothermal setting this is equivalent to showing that $\partial_t \Psi \le 0$ for a closed system. So we replace for this analysis the boundary condition $\mu^j = \overline{\mu}$ in (24) by

$$\partial_{\boldsymbol{n}} \mu^j = 0 \qquad \text{on } \partial\Omega. \tag{29}$$

This ensures that there is no mass flux along $\partial\Omega$.

Looking at the Euler-Lagrange equations derived above, from the stationarity of Ψ with respect to χ, κ and P we immediately get that it is enough to show that

$$\frac{\partial \Psi}{\partial \mu} \cdot \partial_t^h \mu = \int_\Omega \varrho \cdot \partial_t^h \mu \le 0, \tag{30}$$

where all other arguments of Ψ are kept fixed. As a consequence to (14), (12), it holds $\varrho_i \partial_t^h \mu_i = \partial_t^h \varrho_i$ and therefore

$$\frac{\partial \Psi}{\partial \mu} \cdot \partial_t^h \mu = \sum_{i=0}^m \int_\Omega \operatorname{div}(L \nabla \mu_i) - \varrho_i \operatorname{div}(\partial_t^h \varphi)\, dx.$$

Using the divergence theorem and because of $\varphi^j = \varphi^{j-1} = \overline{\varphi}$ on $\partial\Omega$ and (29) the validity of the second law follows.

4. Single slip system and extensions

For a single slip system, the plastic deformation is characterised by vectors $m, n \in \mathbb{R}^3$, $|m| = |n| = 1$ with the slip direction m and the plane normal n. The slip does not change the specific volume of the material, thus $m \cdot n = 0$.

For $Y_{x,D\chi}$ we make the ansatz

$$Y_{x,D\chi}(\xi, \pi, \overline{X}) := |m \cdot \overline{X} n| - \pi + |\xi| \mathcal{X}_{S(D\chi)}(x) - \sigma_Y, \tag{31}$$

where as before $\pi \geqslant 0$. A simpler formula related to (31) was first used in [34]. Equation (31) states a linear hardening law where phase transitions soften the material. We repeat once more that this ansatz is in accordance to the physical picture, see [9] and references therein.

The flow rule (5) becomes for the Lagrange multiplier $\partial_t \Lambda \ge 0$

$$(\partial_t \chi, \partial_t \kappa, P^{-1} \partial_t P) = \partial_t \Lambda \left(\operatorname{sgn}(\xi) \mathcal{X}_{S(D\chi)}(x), -1, \operatorname{sgn}(m \cdot \overline{X} n) m \otimes n \right). \tag{32}$$

Here, $\otimes$ denotes the dyadic product of two vectors, $(m \otimes n)_{ij} = (m_i n_j)_{ij}$. We set $\partial_t \gamma := \operatorname{sgn}(m \cdot \overline{X} n)\, \partial_t \Lambda$ with $\gamma(t=0) = 0$; $\gamma \in \mathbb{R}$ is the slip rate of the slip system. Because $\partial_t \kappa = -\partial_t \Lambda \leqslant 0$ with (32) it follows that $\partial_t \kappa = -|\partial_t \gamma|$.

Also, from (32), $\partial_t P = \partial_t \gamma (Pm) \otimes n$, and, using $m \cdot n = 0$, $\partial_t Pm = 0$. With the initial condition $P(t = 0) = \mathrm{Id}$ we infer $Pm = m$ and thus $\partial_t P = \partial_t \gamma\, m \otimes n$. Together with $P(t = 0) = \mathrm{Id}$, this implies that

$$P = \mathrm{Id} + \gamma m \otimes n. \tag{33}$$

It is immediate that $\det P = 1$ and hence $\det F_{\mathrm{e}} = \det F$.

Direct computations yield the Fenchel conjugate of $Q_{x,D\chi}$ to be

$$\begin{aligned}
&Q^{\star}_{x,D\chi}(\chi', \kappa', \gamma' m \otimes n)\\
&= \sup \left\{ \chi'\xi + \kappa'\pi + \gamma' m \otimes n : \overline{X} \;\middle|\; Y_{x,D\chi}(\xi, \pi, \overline{X}) \leqslant 0,\, \pi \geqslant 0 \right\}\\
&= \sup \big\{ \chi'\xi + \kappa'\pi + \gamma' m \otimes n : \overline{X} \;\big|\\
&\qquad\quad |m \otimes n : \overline{X}| - \pi + |\xi| \mathcal{X}_{S(D\chi)}(x) \leqslant \sigma_Y,\, \pi \geqslant 0 \big\}\\
&= \sup\{ (|m \otimes n : \overline{X}| - \pi + |\xi| \mathcal{X}_{S(D\chi)}(x)) |\gamma'| + (|\gamma'| + \kappa')\pi\\
&\qquad + (|\chi'| - |\gamma'| \mathcal{X}_{S(D\chi)}(x)) |\xi| \;|\\
&\qquad\quad |m \otimes n : \overline{X}| - \pi + |\xi| \mathcal{X}_{S(D\chi)}(x) \leqslant \sigma_Y,\, \pi \geqslant 0 \}\\
&= \begin{cases} \sigma_Y |\gamma'| & \text{if } |\gamma'| + \kappa' \leqslant 0 \text{ and } |\chi'| - |\gamma'| \mathcal{X}_{S(D\chi)}(x) \leqslant 0,\\ \infty & \text{otherwise.} \end{cases}
\end{aligned} \tag{34}$$

With the components $C_{mm} := m \cdot Cm$, $C_{mn} := m \cdot Cn$ of the (right) Cauchy-Green tensor $C := F^T F$, the free energy minimisation (21) becomes for the first time step

$$\begin{aligned}
\Psi(\mu, \chi, \kappa, \varphi, \gamma)(t) = \int_{\Omega} &\psi^{\star}(\mu, \chi) + |D\chi| + U(\sqrt{\det C})\\
&+ \frac{\nu(\chi)}{2} \left(\mathrm{tr} C + 2C_{mn}\gamma + C_{mm}\gamma^2 \right) + \frac{\lambda}{2}\kappa^2 + \sigma_Y |\gamma - \gamma_0| \,\mathrm{d}x\\
&\to \min
\end{aligned}$$

subject to the constraints: (23) on μ and

$$\begin{aligned}
|\gamma - \gamma_0| + \kappa - \kappa_0 &\leqslant 0,\\
|\chi - \chi_0| &\leqslant |\gamma - \gamma_0| && \text{in } S(D\chi_0),\\
\chi &= \chi_0 && \text{in } \Omega \setminus S(D\chi_0).
\end{aligned}$$

Since $\partial_t\kappa \leqslant 0$, minimising $\varPsi$ with respect to κ yields $\kappa = \kappa_0 - |\gamma-\gamma_0|$, leading to the minimisation problem

$$\begin{aligned}
&\varPsi(\mu,\chi,\varphi,\gamma)(t)\\
&= \int_\Omega \psi^\star(\mu,\chi) + |D\chi| + U(\sqrt{\det C})\\
&\qquad + \frac{1}{2}(\nu(\chi)C_{mm}+\lambda)(\gamma-\gamma_0)^2 + \nu(\chi)(C_{mn}+\gamma_0 C_{mm})(\gamma-\gamma_0)\\
&\qquad + (\sigma_Y-\lambda\kappa_0)|\gamma-\gamma_0| + \frac{\nu(\chi)}{2}(C_{mm}\gamma_0^2 + 2C_{mn}\gamma_0 + \mathrm{tr}C) + \frac{\lambda}{2}\kappa_0^2\,\mathrm{d}x\\
&\to \min
\end{aligned}$$

subject to the constraints: (23) on μ and

$$\begin{aligned}
&|\gamma-\gamma_0| \geqslant 1 && \text{in } K(\chi) := \Big\{x\in S(D\chi_0)\ \Big|\ |\chi(x)-\chi_0(x)| = 1\Big\},\\
&\chi = \chi_0 && \text{in } \Omega\setminus S(D\chi_0).
\end{aligned} \tag{35}$$

Let

$$\begin{aligned}
f(\chi,\varphi,\gamma-\gamma_0) := {}&\underbrace{\frac{1}{2}(\nu(\chi)C_{mm}+\lambda)}_{=:c_1(\chi,\varphi)>0}(\gamma-\gamma_0)^2 + \underbrace{\nu(\chi)(C_{mn}+\gamma_0 C_{mm})}_{=:c_2(\chi,\varphi)}(\gamma-\gamma_0)\\
&+ \underbrace{(\sigma_Y-\lambda\kappa_0)}_{=:c_3>0}|\gamma-\gamma_0| + \underbrace{\frac{\nu(\chi)}{2}(C_{mm}\gamma_0^2 + 2C_{mn}\gamma_0 + \mathrm{tr}\,C) + \frac{\lambda}{2}\kappa_0^2}_{=:c_4(\chi,\varphi)}.
\end{aligned}$$

(Note that $c_3 > 0$ as $\sigma_Y > 0$, $\lambda > 0$ and $\kappa \leqslant 0$.) When minimising $\varPsi$ with respect to γ we seek to minimise $f(\chi,\varphi,\cdot)$ subject to (35).

The Cauchy-Green tensor is positive semi-definite. Here we make the stronger assumption that $C_{mm} > 0$. Thus $c_1 > 0$. Consequently $f(\chi,\varphi,\cdot)$ is bounded from below. We leave it to the reader to verify that the minimum is given by

$$f^{\min}(\chi,\varphi) = \begin{cases}
-\frac{(|c_2(\chi,\varphi)|-c_3)_+^2}{4c_1(\chi,\varphi)} + c_4(\chi,\varphi) & \text{in } S(D\chi_0)\setminus K(\chi),\\
-\frac{(|c_2(\chi_0,\varphi)|-c_3)_+^2}{4c_1(\chi_0,\varphi)} + c_4(\chi_0,\varphi) & \text{in } \Omega\setminus S(D\chi_0),\\
c_1(\chi,\varphi) - |c_2(\chi,\varphi)| + c_3 + c_4(\chi,\varphi) & \text{in } K(\chi),
\end{cases}$$

where $(\cdot)_+ := \max(\cdot, 0)$.

Thus we obtain the new minimisation problem

$$\begin{aligned}
\varPsi(\mu,\chi,\varphi)(t) := \int_\Omega \psi^\star(\mu,\chi) + |D\chi| + U(\sqrt{\det C}) + f^{\min}(\chi,\varphi)\,\mathrm{d}x\\
\to \min,
\end{aligned}$$

where μ satisfies (23).

4.1. An example

For illustration of the behaviour of the solution, let $\gamma_0 = \kappa_0 = 0$. This means that we look at the evolution of a single-slip system starting from an ideal elastic material without damage.

We want to study the spatial variations of F, so we consider the family of deformations

$$F(x) = \mathrm{Id} + \frac{\alpha(x)}{2}(n+m) \otimes (n-m), \tag{36}$$

for a function $\alpha : \Omega \to \mathbb{R}$. The ansatz (36) corresponds to a shear under an angle of 45 degrees with respect to the chosen slip system.

For this choice (36) of F we compute $C_{mn} = -\frac{\alpha^2}{2}$, $C_{mm} = 1 - \alpha + \frac{\alpha^2}{2}$. Thus

$$c_1(\chi) = \frac{\nu(\chi)}{2}\left(1 - \alpha + \frac{\alpha^2}{2}\right) + \frac{\lambda}{2}, \qquad c_2(\chi) = -\frac{\nu(\chi)}{2}\alpha^2,$$
$$c_3 = \sigma_Y, \qquad c_4 = \nu(\chi)(3 + \alpha^2).$$

We obtain for $f^{\min}$

$$f^{\min}(\chi,\alpha) = \begin{cases} \nu(\chi)(3+\alpha^2) - \frac{(\frac{\nu(\chi)}{2}\alpha^2 - \sigma_Y)_+^2}{2\left(\nu(\chi)(1-\alpha+\frac{\alpha^2}{2})+\lambda\right)} & \text{in } S(D\chi_0) \setminus K(\chi), \\ \nu(\chi_0)(3+\alpha^2) - \frac{(\frac{\nu(\chi_0)}{2}\alpha^2 - \sigma_Y)_+^2}{2\left(\nu(\chi_0)(1-\alpha+\frac{\alpha^2}{2})+\lambda\right)} & \text{in } \Omega \setminus S(D\chi_0), \\ \nu(\chi)(3+\alpha^2) + \frac{\nu(\chi)}{2}\left(1 - \alpha - \frac{\alpha^2}{2}\right) + \frac{\lambda}{2} + \sigma_Y & \text{in } K(\chi). \end{cases}$$

We study the convexity in α of $f^{\min}$. This is needed for the lower semi-continuity in φ of Ψ – lack of convexity gives rise to the presence of microstructure. It suffices to compute $\frac{\partial^2 f^{\min}}{\partial\alpha^2}$, as $f^{\min}$ is smooth.

Setting $u(\alpha) := 4\nu(2 - 2\alpha + \alpha^2) + 8\lambda$ we compute in $\Omega \setminus K$

$$\frac{\partial^2 f^{\min}}{\partial \alpha^2} = 2\nu + \frac{12\nu^2\alpha^2u^2 + (4\sigma_Y^2 - \nu^2\alpha^4)(u''u - 2u'u') - 8\nu^2\alpha^3uu'}{u^3}.$$

Here $\nu = \nu(\chi)$ in $S(D\chi_0) \setminus K(\chi)$ and $\nu = \nu(\chi_0)$ in $\Omega \setminus S(D\chi_0)$.

A further calculation shows that this is non-negative for λ sufficiently large. Thus (as in the case without phase transitions [10]) hardening opposes the generation of microstructure. In contrast, for λ small, $f^{\min}$ is non-convex in $\Omega \setminus K$ provided α is small.

On the other hand, in $K(\chi)$,

$$\frac{\partial^2 f^{\min}}{\partial \alpha^2} = \frac{3}{2}\nu(\chi). \tag{37}$$

For this case we find that the phase transition has a convexifying effect on the functional. There is no microstructure in the region K of the slip band $S(D\chi_0)$ where the bulk phase has just formed.

We note that the above computations in idealisation state that diffusion does not affect the mechanical properties of the system, i.e. does not influence the occurrence of microstructure. Still, the minimal values of Ψ are affected by the diffusion and this also affects which microstructures are optimal.

5. von Mises yield stress

The finite-strain version of the von Mises yield function criterion reads

$$Y_{D\chi}(\xi,\pi,\overline{X}) := \|\mathrm{dev}\ \mathrm{sym}\overline{X}\| - \sigma_Y - \pi + |\xi|\mathcal{X}_{S(D\chi)}. \tag{38}$$

In this definition, as before, the material constant $\sigma_Y > 0$ is the yield stress, $\pi \geq 0$ and the deviatoric part $\mathrm{dev}(\overline{X})$ of $\overline{X}$ in d space dimensions is given by

$$\mathrm{dev}(\overline{X}) := \overline{X} - \frac{1}{d}\mathrm{tr}(\overline{X})\mathrm{Id}.$$

The symmetrisation of $\overline{X}$ is given by $\mathrm{sym}\overline{X} := \frac{1}{2}(\overline{X}^t + \overline{X})$.

Recall that by (6)

$$Q^\star_{x,D\chi}(c,a,B) = \sup_{(\xi,\pi,\overline{X})}\Big\{\xi c+\pi a+\overline{X}:B\ \Big|\ \|\mathrm{dev}\ \mathrm{sym}\overline{X}\|-\pi+|\xi|\mathcal{X}_{S(D\chi)} \leq \sigma_Y\Big\}.$$

We claim that

$$Q^\star_{x,D\chi}(c,a,B) = \begin{cases}\sigma_Y\|B\| \text{ if } B=B^t,\ \mathrm{tr}(B)=0,\ |c|\leq\|B\|\mathcal{X}_{S(D\chi)},\ \|B\|+a\leq 0,\\ +\infty \quad \text{else.}\end{cases}$$

For the proof of this formula, let us first find necessary conditions for $Q^\star_{x,D\chi}(c,a,B) < \infty$. Choosing $(\xi,\pi,\overline{X}) := \alpha(0,0,\mathrm{Id})$ for arbitrary $\alpha \in \mathbb{R}$ we obtain $\mathrm{tr}(B) = 0$. Similarly, when choosing orthogonal matrices $\overline{X} = -\overline{X}^t$ in the definition of $Q^\star_{x,D\chi}$, we find that $B = B^t$. For $\|B\| \neq 0$ we set $\zeta := \frac{1}{\|B\|}(\sigma_Y + \pi - |\xi|\mathcal{X}_{S(D\chi)})$ and check that $Y_{D\chi}(\xi,\pi,\zeta B) = 0$. Consequently

$$\begin{aligned}\zeta\|B\|^2 + \pi a + \xi c &= \sigma_Y\|B\| + \pi(a + \|B\|) + |\xi|(\mathrm{sgn}(\xi)c - \|B\|\mathcal{X}_{S(D\chi)})\\ &\leq Q^\star_{x,D\chi}(c,a,\zeta B) < \infty.\end{aligned}$$

The formula for $Q^\star_{x,D\chi}$ follows directly from this estimate.

The flow rule (5) becomes

$$(\partial_t\chi, \partial_t\kappa, P^{-1}\partial_t P) = \partial_t\Lambda\Big(\mathrm{sgn}(\xi), -1, \mathrm{sign}(\mathrm{dev}\,\mathrm{sym}\overline{X})\Big).$$

Here we introduced $\mathrm{sign}(A) := A/\|A\|$ if $A \neq 0$ and $\mathrm{sign}(0)$ is the set of all symmetric, trace-free matrices A with $\|A\| \leq 1$. This gives $\mathrm{tr}(P^{-1}\partial_t P) = 0$ which implies with $P(t=0) = \mathrm{Id}$ the condition $\det P = 1$.

A main obstruction to the construction of a time-discrete scheme is the condition $\det P = 1$ which has to be guaranteed by the choice on $d_t^h(P)$. The standard approach is

$$d_t^h(P) := \log(P_0^{-1} P). \tag{39}$$

This expression is well-defined as long as $P_0^{-1}P$ is symmetric and positive definite. Ansatz (39) is meaningful as with symmetric and trace-free $H := d_t^h(P)$ it follows $P = P_0 \exp(H)$ which gives as desired $\det P = 1$ if $\det P_0 = 1$.

The free energy minimisation (21) reads now

$$\Psi(\mu,\chi,\kappa,\varphi,P) = \int_\Omega \Big[|D\chi| + U(\det F) + \frac{\nu(\chi)}{2}\mathrm{tr}[P^t C P] + \psi^\star(\mu,\chi) + \frac{\lambda}{2}\kappa^2 + \sigma_Y \| \log(P_0^{-1}P)\| \Big]\, \mathrm{d}x \to \min$$

where μ fulfils (23) and subject to the constraints

$$\mathrm{tr}[\log(P_0^{-1}P)] = 0, \qquad P_0^{-1}P = (P_0^{-1}P)^t,$$
$$\|\log(P_0^{-1}P)\| + \kappa - \kappa_0 \le 0, \qquad |\chi - \chi_0| \le \|\log(P_0^{-1}P)\| \mathcal{X}_{S(D\chi_0)}.$$

Elimination of the second and third constraint yields after optimisation with respect to κ

$$\kappa = \kappa_0 - \|\log(P_0^{-1}P)\|.$$

Thus we obtain with $C = (D\varphi)^t D\varphi$ the simplified minimisation problem

$$\Psi(\mu,\chi,\varphi,P) = \int_\Omega \Big[|D\chi| + U(\sqrt{\det C}) + \psi^\star(\mu,\chi) + \frac{\nu(\chi)}{2}\mathrm{tr}[P^t C P] + \frac{\lambda}{2}\kappa_0^2 + \frac{\lambda}{2}\|\log(P_0^{-1}P)\|^2 + (\sigma_Y - \lambda\kappa_0)\|\log(P_0^{-1}P)\| \Big]\, \mathrm{d}x \to \min$$

subject to the condition (23) on μ and subject to

$$\mathrm{tr}[\log(P_0^{-1}P)] = 0, \qquad |\chi - \chi_0| \le \|\log(P_0^{-1}P)\| \mathcal{X}_{S(D\chi_0)}.$$

Introducing the symmetric matrix H via the equation $P = P_0\exp(H)$ and replacing the optimisation with respect to P by an optimisation with respect to H, we obtain

$$\Psi(\mu,\chi,\varphi,H) = \int_\Omega \Big[|D\chi| + U(\sqrt{\det C}) + \frac{\lambda}{2}\kappa_0^2 + \frac{\lambda}{2}\|H\|^2 + (\sigma_Y - \lambda\kappa_0)\|H\| + \psi^\star(\mu,\chi) + \frac{\nu(\chi)}{2}\mathrm{tr}[\exp(H) P_0^t C P_0 \exp(H)] \Big]\, \mathrm{d}x \to \min$$

subject to (23) and to

$$\mathrm{tr}(H) = 0, \qquad |\chi - \chi_0| \le \|H\| \mathcal{X}_{S(D\chi_0)}.$$

As in Section 4 we study this problem analytically to find out whether there is a convexifying effect of the phase transition within K. We consider local spatial fluctuations in F for the choice

$$F(x) = \mathrm{Id} + \alpha(x)\, n \otimes n,$$

where $\alpha \in \mathbb{R}$, $x \in \Omega$ and n is an arbitrary unit vector. Due to the isotropy of Ψ, the results will not depend on the particular choice of n.

Like in Section 4 we assume $\kappa_0 = 0$ and $P_0 = \mathrm{Id}$ and introduce the 'flip set' $K := \{x \in S(D\chi_0) \,|\, |\chi_0(x) - \chi(x)| = 1\}$ as that subset of Ω where the constraint is active.

We qualitatively study the behaviour of Ψ in 2D writing $H = \begin{pmatrix} u & v \\ v & -u \end{pmatrix}$ for $u, v \in \mathbb{R}$. So we have

$$\Psi(\alpha) = \inf_{\mu,\chi} \inf_{H=H^t,\, \mathrm{tr}(H)=0} \int_\Omega \Big[|D\chi| + U(\sqrt{\det C}) + \frac{\lambda}{2}\|H\|^2 + \sigma_Y \|H\| \\ + \psi^\star(\mu,\chi) + \frac{\nu(\chi)}{2} \mathrm{tr}\Big(\exp(H) C \exp(H)\Big)\Big]\, \mathrm{d}x.$$

The optimisation with respect to μ is as before understood subject to constraint (23). The minimisation with respect to H immediately gives $v = 0$.

For U we make the standard choice

$$U(d) := \frac{\tilde{\nu}(\chi)}{4} d^2 - \frac{\tilde{\nu}(\chi) + 2\nu(\chi)}{2} \log(d). \tag{40}$$

In the infinitesimal setting, the ansatz (40) reduces to an isotropic elastic material with Lamé parameters ν and $\tilde{\nu}$. For the analysis we set $\tilde{\nu} \equiv 0$.

On K we have $\|H\| = 1$. This implies

$$\begin{aligned} \mathrm{tr}\Big[\exp(H) C \exp(H)\Big] &= \mathrm{tr}\Big[\sum_{j=0}^\infty \frac{1}{j!(\sqrt{2})^j} \begin{pmatrix} 1 & 0 \\ 0 & (1+\alpha)^2 \end{pmatrix} \sum_{j=0}^\infty \frac{1}{j!(\sqrt{2})^j}\Big] \\ &= \exp(2\sqrt{2}) \Big[1 + (1+\alpha)^2\Big]. \end{aligned}$$

Consequently

$$\Psi(\alpha)\Big|_K = \inf_\mu \inf_{\chi \in BV(\Omega)} \int_K \Big[|D\chi| - \nu(\chi) \log|1+\alpha| + \frac{\lambda}{2} + \sigma_Y \\ + \psi^\star(\mu,\chi) + \frac{\nu(\chi)}{2} \exp(2\sqrt{2}) \Big(1 + (1+\alpha)^2\Big)\Big]\, \mathrm{d}x$$

implying that $\alpha \mapsto \Psi(\alpha)|_K$ is convex.

On $\Omega \setminus K$, we observe the identity

$$\begin{aligned} \mathrm{tr}[\exp(H) C \exp(H)] &= \mathrm{tr}\left[\exp(2H) \begin{pmatrix} (1+\alpha)^2 & 0 \\ 0 & 1 \end{pmatrix}\right] \\ &= (1+\alpha)^2 \exp(2u) + \exp(-2u). \end{aligned}$$

We conclude that the free energy minimisation becomes

$$\Psi(\alpha)\Big|_{\Omega\setminus K} = \inf_{\chi,\,\mu,\,u} \int\limits_{\Omega\setminus K} \Big[|D\chi| - \nu(\chi)\log|1+\alpha| + \lambda u^2 + \sqrt{2}\sigma_Y |u| + \psi^\star(\mu,\chi) + \frac{\nu(\chi)}{2}\Big((1+\alpha)^2\exp(2u) + \exp(-2u)\Big)\Big]\,\mathrm{d}x.$$

The Euler-Lagrange equation for the minimising u is

$$2\lambda u + \sqrt{2}\sigma_Y \operatorname{sgn}(u) + \nu(\chi)\Big((1+\alpha)^2\exp(2u) - \exp(-2u)\Big) = 0. \tag{41}$$

The explicit analytic solution of (41) is lengthy. Instead, Figure 1 shows the results of some numerical computations for $\nu(\chi) \equiv 2$, $h = 0.001$ and $\chi \equiv 1$ in Ω, i.e. in the absence of phase transitions. Concerning the dependence on α, the results coincide with those reported in [10]: For λ large enough, it holds $\frac{\partial^2 \Psi}{\partial \alpha^2}\Big|_{\Omega\setminus K} \geq 0$ and there is a regularising effect of hardening on the formation of microstructure. For λ close to 0, we have that Ψ is non-convex.

In summary, we observe the same behaviour as in Section 4: Lack of convexity of $\alpha \mapsto \Phi(\alpha)$ occurs in $\Omega \setminus K$ and gives rise to the presence of microstructure, whereas in the flip set K the convexity of Φ in α prohibits oscillations on a small scale.

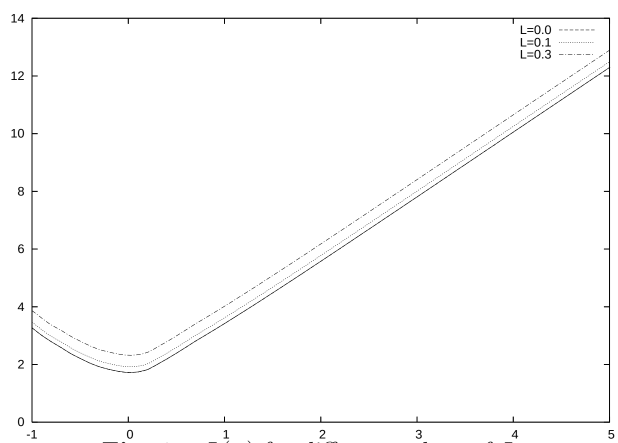

Fig. 1. $\Psi(\alpha)$ for different values of L

Figure 1 shows in particular the dependence of the energy on diffusion, i.e. for different L. The larger the value of L, the bigger the inflow of mass given by $\int_\Omega \operatorname{div}(L\nabla\mu) = \int_{\partial\Omega} L\nabla\overline{\mu}\cdot\boldsymbol{n}$, and due to (15), there is a monotone relationship between ϱ^j and μ^j.

6. Discussion

Based on rate-independent finite-strain elastoplasticity, a theory for phase transitions in solids respecting hardening and diffusional effects was developed, where the stored mechanical energy W depends additionally on a phase parameter χ. As main result, a waiting time phenomenon was derived and it was shown that microstructure does not occur in those regions where a phase transformation has just taken place.

Possible applications of the derived model are materials with a manufactured structure variation on the macroscopic scale, especially composites like the metal-intermetallic laminates, [36] and [37], or certain ceramic-metal ('cermet') materials, see for instance [24].

When studying mechanical systems, the effect of diffusion may be negligible in many cases, but not always. The experiments in [25] demonstrate the influence of diffusion on a phase boundary. Furthermore, diffusion leads to a shift in the actual position of the minimisers of the free energy. This may result in topological changes in the occurring microstructure. The optical microscopy on NiTi specimen in [7] gives indications to this phenomenon for shape memory materials.

Finally, it is noteworthy to observe the following simplification in the derivation of our model: The decomposition (1) and ansatz (2) do not keep track of the lattice orientation at time t. This is completely inadequate to model materials with damage, or as an extreme case, lattice recrystallisation. In our model, neglecting the lattice orientation leads to a non-physical interfacial surface energy. The term $\int_\Omega |D\chi|$ stands for an isotropic surface energy, but neglects the different lattice orientations on both sides of the interface which lead to geometric misfits and alter the interfacial energy.

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