

Notes on strain gradient plasticity: Finite strain covariant modelling and global existence in the infinitesimal rate-independent case.

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Abstract

We propose a model of finite strain gradient plasticity including phenomenological Prager type linear kinematical hardening and nonlocal kinematical hardening due to dislocation interaction. Based on the multiplicative decomposition a thermodynamically admissible flow rule for F_p is described involving as plastic gradient $\text{Curl } F_p$. The formulation is covariant w.r.t. superposed rigid rotations of the reference, intermediate and spatial configuration but the model is not spin-free due to the nonlocal dislocation interaction and cannot be reduced to a dependence on the plastic metric $C_p = F_p^T F_p$.

The linearization leads to a thermodynamically admissible model of infinitesimal plasticity involving only the Curl of the non-symmetric plastic distortion p . Linearized spatial and material covariance under constant infinitesimal rotations is satisfied.

Uniqueness of strong solutions of the infinitesimal model is obtained if two non-classical boundary conditions on the plastic distortion p are introduced: $\dot{p} \cdot \tau = 0$ on the microscopically hard boundary $\Gamma_D \subset \partial\Omega$ and $[\text{Curl } p] \cdot \tau = 0$ on the microscopically free boundary $\partial\Omega \setminus \Gamma_D$, where τ are the tangential vectors at the boundary $\partial\Omega$. Moreover, we show that a weak reformulation of the infinitesimal model allows for a global in-time solution of the corresponding rate-independent initial boundary value problem. The method of choice are a formulation as a quasivariational inequality with symmetric and coercive bilinear form. Use is made of new Hilbert-space suitable for dislocation density dependent plasticity.

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1 Introduction

This article addresses the modelling and mathematical analysis of a **geometrically linear gradient plasticity** model. There is an abundant literature on gradient plasticity formulations, in most cases letting the yield-stress depend also on some higher derivative of a scalar measure of accumulated plastic distortion [36, 10, 13]. Experimentally, the dependence of the yield stress on plastic gradients is well-documented [12]. Several experimental facts testify to the length scale dependence of materials: the **Hall-Petch scaling**¹ relates the grain size in polycrystals to the yield stress: $\sigma_y = \sigma_y^0 + \frac{k^+}{\sqrt{\text{grainsize}}}$.

The **Taylor scaling** relates the flow stress σ_y to the dislocation density: $\sigma_y = \sigma_y^0 + k^+ \|\text{Curl } F_p\|$. It is also known that the thinner the grains, the stiffer the material gets. As a rule one may say: the smaller the sample the stiffer it gets (while unbounded stiffness can be excluded from atomistic calculations).

From a numerical point of view the incorporation of plastic gradients serves the purpose of removing the mesh-sensitivity, either in the softening case, or, more difficult to observe numerically, already in classical Prandtl-Reuss plasticity (shear bands and slip lines with ill-defined band width).

The incorporation of a length scale, which is a natural by-product of gradient plasticity, has the potential to remove the mesh sensitivity. The presence of the internal length scale causes the localization zones to have finite width. It makes possible the analysis of failure problems in which strain localization into shear bands occurs. However, the actual length scale of a material is difficult to establish experimentally and theoretically and remains basically an open question as is the determination of other additionally appearing material constants. It is also not entirely clear, how the shear band width depends on the characteristic length.

The finite strain model we propose is based on the multiplicative decomposition of the deformation gradient and does not modify the yield stress directly but incorporates, motivated by mechanism-based single crystal plasticity, the dislocation density into the thermodynamic potential. The corresponding flow rule can be extracted in a non-standard way, based on the development in Maugin [28]. Models, similar in spirit to our formulation, may be found in [30, 25]. The necessary re-interpretation of the second law of thermodynamics can be found, e.g., in [28, 27]. This development is based on ideas initially proposed in [37], cf. [49, 11]. In contrast to [30, 25] we evaluate the extended dissipation principle in a more relaxed sense.

While gradient plasticity seems to be of high current interest [15, 18, 17] we have not been able to locate any mathematical study of the time continuous higher gradient plasticity problem, apart for Reddy [50] treating a geometrically linear model of Gurtin [15], different from our proposal.²

Gurtin includes F_p in the free energy and takes free variations with respect to F_p , leading to a model with additional balance equations for microforces, similar, e.g., to a Cosserat or Toupin-Mindlin type model. In contrast, in our model F_p and thence $\text{Curl } F_p$

¹There is also a reverse Hall-Petch scaling for very small grains in the nano-range.

²In Reddys analytical treatment of the corresponding infinitesimal model strong assumptions on the presence of the full plastic gradient are introduced in the dependence of the yield stress on the plastic gradients in order to show existence and uniqueness. His model features purely symmetric plastic strains.

is treated as an inner variable included only in the thermodynamic potential, leading to evolution equations for F_p of degenerate parabolic type.

In Mielke&Müller [34] the time-incremental finite-strain problem is investigated. It is shown that once the update potential for one time step is established and known to be properly coercive and polyconvex as a function of F_e in the multiplicative decomposition of the deformation gradient, then, adding a regularizing term depending on $\text{Curl } F_p$ is indeed enough to show existence of minimizers in this update problem for the new deformation and the new plastic variable.³ Adding a $\text{Curl } F_p$ -related term to the time-incremental problem has been suggested in [47] for the description of subgrain dislocation structures. It seems therefore necessary to investigate the general structure of these class of gradient plasticity models, mainly with respect to their regularizing power, also in conjunction with large scale parallel implementations. Focussing therefore on localization limiters we show well-posedness of a model which includes the dislocation energy density and local linear Prager kinematic hardening. In the large scale (classical) limit the model turns into classical Prandtl-Reuss plasticity with linear kinematic hardening.

As far as classical rate-independent elasto-plasticity is concerned we remark that global existence for the displacement has been shown only in a very weak, measure-valued sense, while the stresses could be shown to remain in $L^2(\Omega)$. For this results we refer for example to [3, 9, 52]. If hardening or viscosity is added, then global classical solution are found see e.g. [1, 8, 7]. A complete theory for the classical rate-independent case remains elusive, see also the remarks in [9]. It is therefore hoped, that including plastic gradients in the formulation will regularize the problem and lead to a well-posed model. This is what we will make rigourously.

Our contribution is organized as follows: first, we present a basic modelling of multiplicative gradient plasticity and show that the formulation is thermodynamically consistent in an extended sense. We impose sufficient conditions for the insulation condition to hold. No conditions inside the bulk between elastic and plastic parts are imposed. Then we motivate full spatial, intermediate and referential covariance under constant rotations. Thus our finite strain model is objective and isotropic w.r.t. both the reference configuration and the intermediate configuration. Nevertheless, the model cannot be reduced to depend on the plastic metric $C_p = F_p^T F_p$ only because of the presence of plastic gradients.

Subsequently, we repeat the derivation of the model in the geometrically linear context. Strong solutions of the obtained model with general monotone, non-associative flow-rule together with suitable boundary conditions on the non-symmetric infinitesimal plastic distortion p can be shown to be unique. In the classical case with rate-independent flow rule coming from the subdifferential of a convex domain in stress-space (Prandtl-Reuss) we are able to reformulate the problem as a mixed variational inequality and to show existence and uniqueness in a suitably defined non-standard Hilbert-space. The relevant notation is found in the appendix.

³It is noteworthy that the update problem in [34] is a two-field minimization problem for (φ, F_p) in the spirit of a micromorphic model [39] with a very special coupling between the different fields φ and F_p . Polyconvexity in F_e alone is not sufficient to obtain existence by Ball's method since F_e is not a gradient, but the term $\text{Curl } F_p$ provides additional compactness in the spirit of Murat/Tartars method.

2 Thermodynamics

2.1 Extended statement of the second law of thermodynamics

The following treatment is based on ideas apparently first proposed by I. Müller in 1967 [37] in an investigation of the form of the entropy inequality. Müller introduced an **extra entropy flux** into the second law of thermodynamics (Clausius-Duhem inequality) which only has to satisfy natural invariance conditions. Elaborating on these ideas, Maugin [28, Eq.2.14] considered gradient dependent plasticity models within a general treatment of **thermodynamics with internal variables (T.I.V)**. There he introduced the idea of this "extra entropy flux" to account for the hardening/softening diffusion process. This causes the Clausius-Duhem inequality to encompass an extra term restricted (only) by the condition that the dissipation density takes a suitable bilinear format. A recent account can be found in [27] which we adapt freely for our purpose.

Assume constant density $\varrho > 0$ and constant temperature ($\Theta = \text{const.}$, isothermal process) throughout. Let W be the Helmholtz free energy, depending on $\nabla\varphi$ and a set of internal variables ζ . Then the classical non-localized statement of the **second law of thermodynamics** reads: $\forall \mathcal{V} \subseteq \Omega$

$$\int_{\mathcal{V}} \underbrace{\langle S_1(F(t), \zeta(t)), \nabla\varphi_t \rangle - \varrho \frac{d}{dt} W(\nabla\varphi(t), \zeta(t))}_{\mathcal{D}} dV \geq 0 \Leftrightarrow \quad (2.1)$$

$$\int_{\mathcal{V}} \underbrace{\frac{d}{dt} W(\nabla\varphi(t_0), \zeta(t))}_{\leq 0 \text{ reduced dissipation inequality}} dV \leq 0 \quad \text{at frozen } t_0 \in \mathbb{R},$$

with $\mathcal{D} \geq 0$ the **non-negative dissipation** due to the evolution of the inner variables. For sufficiently smooth integrands one obtains by localization the classical statement of the local **reduced dissipation inequality**

$$\forall x \in \Omega \quad \forall t \in \mathbb{R} : \quad \frac{d}{dt} W(\nabla\varphi(x, t_0), \zeta(x, t)) \leq 0. \quad (2.2)$$

Maugin [27] extends this classical definition to cover also models depending on gradients of internal variables, i.e., models where also $\nabla_x \zeta$ is involved. The extended nonlocal version can be read as: $\forall \mathcal{V} \subseteq \Omega$

$$\int_{\mathcal{V}} \underbrace{\langle S_1(F(t), \zeta(t), \nabla\zeta(t)), \nabla\varphi_t \rangle - \varrho \frac{d}{dt} W(\nabla\varphi(t), \zeta(t), \nabla\zeta(t)) + \text{Div } q(\nabla\varphi, \zeta, \nabla\zeta)}_{\mathcal{D}^{\text{nlc}}} dV \geq 0 \Leftrightarrow$$

$$\int_{\mathcal{V}} \frac{d}{dt} W(\nabla\varphi(t_0), \zeta(t), \nabla\zeta(t)) - \text{Div } q(\nabla\varphi, \zeta, \nabla\zeta) dV \leq 0 \quad \text{at frozen } t_0 \in \mathbb{R}, \quad (2.3)$$

where the **extra entropy flux** q may be chosen suitably.⁴ Again, after localization for smooth enough integrands, one is left with the **extended reduced dissipation**

⁴Maugin writes [p.99][27]: "...used the trick to select k (the extra entropy flux) in such a form as to eliminate any true divergence term in the dissipation inequality.

inequality $\forall x \in \Omega \forall t \in \mathbb{R}$:

$$\frac{d}{dt} W(\nabla\varphi(x, t_0), \zeta(x, t), \nabla\zeta(x, t)) - \text{Div } q(\nabla\varphi(x, t), \zeta(x, t), \nabla\zeta(x, t)) \leq 0. \quad (2.4)$$

A major advantage of the new condition (2.3) is its efficiency in deriving evolution equations for the inner variables.

2.2 A priori energy inequality

The condition (2.4) does not make a statement as far as boundary conditions for the internal variables ζ are concerned and indeed Maugin does not propose such conditions. However, for materials which depend on gradients of internal variables this question needs to be addressed. We propose as an additional condition the satisfaction of an energy inequality over the bulk.⁵ We **require that the rate of change of the free energy is bounded by the power of external forces**, i.e.,

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} W(\nabla\varphi(x, t), \zeta(x, t), \nabla\zeta(x, t)) dV &\leq \int_{\Omega} \langle f(x, t), \varphi_t(x, t) \rangle dV \\ &+ \int_{\partial\Omega} \langle \varphi_t(x, t), S_1(\nabla\varphi(x, t), \zeta(x, t), \nabla\zeta(x, t)) \cdot \vec{n} \rangle dS. \end{aligned} \quad (2.6)$$

The condition (2.6) allows us to obtain the **energy inequality**

$$\begin{aligned} \int_{\Omega} W(\nabla\varphi(x, t), \zeta(x, t), \nabla\zeta(x, t)) dV &\leq \int_{\Omega} W(\nabla\varphi(x, 0), \zeta(x, 0), \nabla\zeta(x, 0)) dV \\ &+ \int_0^t \int_{\Omega} \langle f(x, t), \varphi_t(x, t) \rangle dV dt \\ &+ \int_0^t \int_{\partial\Omega} \langle \varphi_t(x, t), S_1(\nabla\varphi(x, t), \zeta(x, t), \nabla\zeta(x, t)) \cdot \vec{n} \rangle dS dt. \end{aligned} \quad (2.7)$$

(The difference to equality in (2.7) is the time-integrated positive dissipation in Mielke [32]) Since⁶

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} W(\nabla\varphi(x, t), \zeta(x, t), \nabla\zeta(x, t)) dV &= \int_{\Omega} \langle f, \varphi_t \rangle dV + \int_{\partial\Omega} \langle \varphi_t, S_1 \cdot \vec{n} \rangle dS \\ &+ \int_{\Omega} \langle D_{\zeta} W - \text{Div } D_{\nabla\zeta} W, \frac{d}{dt} \zeta \rangle dV + \int_{\partial\Omega} \langle \frac{d}{dt} \zeta, D_{\nabla\zeta} W \cdot \vec{n} \rangle dS, \end{aligned} \quad (2.8)$$

inequality (2.7) will be satisfied if,

$$\int_{\Omega} \langle D_{\zeta} W - \text{Div } D_{\nabla\zeta} W, \frac{d}{dt} \zeta \rangle dV + \int_{\partial\Omega} \langle \frac{d}{dt} \zeta, D_{\nabla\zeta} W \cdot \vec{n} \rangle dS \leq 0. \quad (2.9)$$

⁵This is the same as postulating the classical Clausius-Duhem inequality over the bulk, i.e.,

$$\int_{\Omega} \langle S_1, F_t \rangle - \rho \frac{d}{dt} W(F(x, t), \zeta(x, t), \nabla\zeta(x, t)) dV \geq 0, \quad (2.5)$$

i.e., the global rate of change of internal energy is bounded by the power supplied by external forces.

⁶Use $\text{Div } S_1 = -f$.

This in turn is guaranteed if, e.g.,

$$\begin{aligned} \frac{d}{dt}\zeta &= \mathbf{f} \left(\underbrace{-[D_\zeta W - \text{Div } D_{\nabla\zeta} W]}_{\Sigma} \right), \quad \langle \mathbf{f}(X), X \rangle \geq 0, \quad x \in \Omega \\ D_{\nabla\zeta} W \cdot \vec{n} &= 0, \quad x \in \partial\Omega \setminus \Gamma_D \quad \text{micro-free condition,} \\ \dot{\zeta} &= 0, \quad x \in \Gamma_D \quad \text{micro-hard condition.} \end{aligned} \quad (2.10)$$

Note that in the local model (absence of gradients) no possibility for boundary conditions on ζ arises. Requiring simply

$$\int_{\partial\Omega} \left\langle \frac{d}{dt}\zeta, D_{\nabla\zeta} W \cdot \vec{n} \right\rangle dS = \int_{\Omega} \text{Div} \left(D_{\nabla\zeta} W^T \cdot \frac{d}{dt}\zeta \right) dV = 0, \quad \text{insulation condition} \quad (2.11)$$

can be interpreted as **energy insulation condition** on the internal variable in the bulk to the outer world which means that **no nonlocal energy exchange across the external boundary is possible**. Note that (2.10) is stronger than the local insulation condition contrary to (2.11) which itself is sufficient for (2.9) and thence (2.7). The choice between the different boundary conditions which kill the appearing divergence term may be guided by taking the weakest condition which still allows for uniqueness of classical solutions. Such a motivation has been pursued in [18, 8.1]. The different boundary conditions leading to the insulation condition can be subsumed, in the language of Gurtin, as microscopically powerless boundary conditions. In [49], following [11], a much more restrictive set of condition on the additional flux is required, needing boundary conditions also inside the body Ω between plastified regions and elastic regions. The numerical implementation of such conditions is cumbersome.

3 The finite strain gradient plasticity model

3.1 The multiplicative decomposition

It is appropriate to start with a geometrically exact development and to subsequently linearize the kinematical relations in order to obtain our nonlinear gradient plasticity model in the geometrically linear setting. Thus consider the well-known multiplicative decomposition [21, 22, 24, 20] of the deformation gradient $F = \nabla\varphi$ into elastic and plastic parts

$$F = F_e \cdot F_p. \quad (3.1)$$

Recall that while $F = \nabla\varphi$ is a gradient, neither F_e nor F_p need to be gradients themselves. In this decomposition, usually adopted in **single crystal plasticity**, F_e represents **elastic lattice stretching and elastic lattice rotation** while F_p represents local deformation of the crystal due to **plastic rearrangement by slip on glide planes**. In the single crystal case one usually assumes this split to be of the form

$$F_p : T_x \Omega_{\text{ref}} \mapsto T_x \Omega_{\text{ref}}, \quad F_e : T_x \Omega_{\text{ref}} \mapsto T_{\varphi(x)} \Omega_{\text{act}}, \quad F : T_x \Omega_{\text{ref}} \mapsto T_{\varphi(x)} \Omega_{\text{act}}, \quad (3.2)$$

moreover, F_p is viewed as completely constitutively determined by the flow rule for slip on preferred glide planes. In a more phenomenological, polycrystalline model such a constitutive assumption is not mandatory. Here, we consider the split (3.1) rather as a kinematical decomposition. See [4] for an altogether alternative axiomatic approach for the definition of a plastic transformation for materials with isomorphic elastic ranges.

Remark 3.1 (Necessity for covariance requirements)

In all of the following the reader should bear in mind that we restrict our modelling proposal to a fully isotropic setting. From an application oriented view this might seem unrealistic. However, our point is that if anisotropies of whatever kind are to be included they should appear explicitly through the appearance of additional structural tensors reflecting the given symmetries of the material. If this is not done but the formulation is not fully covariant then one introduces carelessly anisotropic behaviour which lacks any real physical basis, cf. [26, p.220].

3.2 The plastic indifference of the elastic response

In all of the following we concentrate on the hyperelastic formulation of finite strain plasticity, i.e., we are concerned with finding the appropriate energy storage terms governing the elastic and plastic behaviour. In general, we assume that the total stored energy can be expressed as

$$W(F, F_p, \text{Curl } F_p) = \underbrace{W_e(F, F_p)}_{\text{elastic energy}} + \underbrace{W_{\text{ph}}(F_p)}_{\text{linear kinematical hardening}} + \underbrace{W_{\text{curl}}(F_p, \text{Curl } F_p)}_{\text{dislocation entangling}}. \quad (3.3)$$

Here, the local hardening potential W_{ph} is a purely phenomenological energy storage term formally consistent with a Prager type constant linear hardening behaviour. The dislocation potential W_{curl} instead is a microscopically motivated storage term due to dislocation entangling which is the ultimate physical reason for any hardening behaviour.

A crucial requirement in finite strain plasticity is the **plastic indifference**⁷ condition [32]. By this we mean that the elastic response of the material, governed by the elastic strain energy part, is invariant w.r.t. arbitrary previous plastic deformation F_p^0 . This means that

$$\forall F_p \in GL^+(3) : W_e(F, F_p) = W_e(F F_p^0, F_p F_p^0). \quad (3.4)$$

Using (3.4) it is easily seen, by specifying $F_p^0 = F_p^{-1}$, that

$$W_e(F, F_p) = W_e(F F_p^{-1}, \mathbb{1}) = W_e(F_e). \quad (3.5)$$

Thus plastic indifference is a constitutive statement about the elastic response and not a fundamental physical invariance law. Plastic indifference reduces the elastic dependence of W_e on F_e alone. It is based on the experimental evidence that unloading and consecutive loading below the yield limit has the same elastic response as the initial virgin

⁷In [4] conceptually the same is expressed by postulating isomorphic elastic ranges.

response.

Remaining in the context of finite strain plasticity, we propose, following Miehe [31] and Bertam [4] a model based on evolution equations for F_p and not on a plastic metric C_p . In order to adapt the micromechanically motivated multiplicative decomposition to a phenomenological description, one usually includes an **assumption on the plastic spin**, i.e. $\text{skew}(F_p \frac{d}{dt} F_p^{-1}) = 0$, a no-spin multiplicative plasticity model based on F_p results but we will refrain from imposing such a condition.

Many of the existing gradient plasticity theories do not involve plastic rotations either, however, Gurtin/Anand [17] note: "unless the plastic spin is (explicitly) constrained to be zero, constitutive dependencies on the Burgers tensor necessarily involve dependencies on the (infinitesimal) plastic rotation."

Since rate-dependence of most metals at room temperature is very small, we limit therefore our consideration to the rate-independent case.

3.3 Illustration of the kinematical multiplicative decomposition based on the chain rule

For illustration purposes let us introduce symbolically the **compatible reference configuration** Ω_{ref} , the **fictitious compatible intermediate configuration** Ω_{int} and the **compatible deformed configuration** Ω_{act} together with mappings

$$\begin{aligned} \Psi_p : x \in \Omega_{\text{ref}} \subset \mathbb{E}^3 &\mapsto \Psi_p(\Omega_{\text{ref}}) = \Omega_{\text{int}} \subset \mathbb{E}^3, & \Psi_e : \eta \in \Omega_{\text{int}} \subset \mathbb{E}^3 &\mapsto \Omega_{\text{act}} \subset \mathbb{E}^3, \\ \varphi : x \in \Omega_{\text{ref}} \subset \mathbb{E}^3 &\mapsto \Omega_{\text{act}} \subset \mathbb{E}^3, \\ \varphi(x) &= \Psi_e(\Psi_p(x)), & \nabla_x \varphi(x) &= \nabla_\eta \Psi_e(\Psi_p(x)) \nabla_x \Psi_p(x) = F_e(x) F_p(x). \end{aligned} \quad (3.6)$$

This means that we have simply realized the total deformation by two subsequent compatible deformations.

3.4 Referential isotropy of material response

Many polycrystalline materials, in particular many metals, can be considered, even after plastically deforming (but before significant texture development occurs) to behave (at least approximately) elastically isotropic. Restricting ourselves to such materials in this work, we assume that the total stored energy W is isotropic with respect to the intermediate configuration, moreover, it will turn out that the Prager linear kinematic hardening potential W_{ph} must be an isotropic function of $C_p = F_p^T F_p$. However, we need to clarify in what sense a gradient plasticity model can be considered to be isotropic.

There is agreement in the literature as far as the meaning of elastic isotropy or isotropy w.r.t. the intermediate configuration is concerned. In this case the elastically stored energy function should be isotropic w.r.t. rotations of the intermediate configuration, i.e.,

$$W_e(F_e \bar{Q}) = W_e(F_e) \quad \forall \bar{Q} \in \text{SO}(3). \quad (3.7)$$

Concerning the determination of the plastic distortion F_p , following Maugin [29, p. 110], it should hold for referentially isotropic materials without plastic gradients, that, given initial conditions

$$F_p(x, 0) \quad \text{versus} \quad F_p(x, 0) \overline{Q}^T, \quad (3.8)$$

differing only by one constant proper rotation $\overline{Q}^T \in \text{SO}(3)$, that the respective solutions of the model, at all later times $t \in \mathbb{R}$ are

$$F_p(x, t) \quad \text{versus} \quad F_p(x, t) \overline{Q}^T. \quad (3.9)$$

Maugin [29, p. 110] calls this **G-covariance**. For full isotropy w.r.t. the reference configuration the material symmetry group is $\text{SO}(3)$. We note that our "plastic distortion rate" $F_p \frac{d}{dt}[F_p^{-1}]$ is form-invariant under $F_p \rightarrow F_p \overline{Q}^T$. It remains then to show that our model will satisfy a suitably extended version of (3.9), taking plastic gradients into account.

Let us refer to **referential isotropy** if the model is form invariant under $(F, F_e, F_p) \rightarrow (F\overline{Q}, F_e, F_p\overline{Q})$, i.e., if (F, F_e, F_p) is a solution, then $(F\overline{Q}, F_e, F_p\overline{Q})$ is a solution to rotated data. Since F_e is left unaltered we see that the referential isotropy condition does not restrict the elastic response of the material but restricts our Prager hardening potential to a functional dependence of the form

$$W_{\text{ph}}(F_p\overline{Q}) = W_{\text{ph}}(F_p) \quad \forall \overline{Q} \in \text{SO}(3) \quad \Rightarrow \quad W_{\text{ph}}(F_p) = \widehat{W}_{\text{sh}}(F_p F_p^T). \quad (3.10)$$

In order to motivate the restrictions of isotropy for the gradient plasticity model we have to review the basic principles underlying the issue of isotropic response. Thus in classical hyperelastic finite-strain elasticity isotropy is defined as the form-invariance of the free-energy under a rigid rotation of the coordinate system. Consider the problem

$$\int_{\Omega} W(\nabla\varphi(x)) \, dx \mapsto \min. \quad \varphi, \quad (3.11)$$

for $\varphi : \Omega_{\text{ref}} \subset \mathbb{R}^3 \mapsto \mathbb{R}^3$. Consider a transformed coordinate system, the transformation being given by a diffeomorphism

$$\zeta : \Omega_{\text{ref}} \mapsto \zeta(\Omega_{\text{ref}}) = \Omega^*, \quad \zeta(x) = \xi. \quad (3.12)$$

By the transformation formula for integrals the problem (3.11) can be transformed to this new configuration. We define the same function φ expressed in new coordinates

$$\varphi^*(\zeta(x)) := \varphi(x) \quad \Rightarrow \quad \nabla_{\xi}\varphi^*(\zeta(x)) \nabla\zeta(x) = \nabla\varphi(x) \quad (3.13)$$

and

$$\int_{\xi \in \Omega^*} W(\nabla_{\xi}\varphi^*(\xi) \nabla_x\zeta(\zeta^{-1}(\xi))) \det[\nabla_x\zeta^{-1}] d\xi \mapsto \min. \quad \varphi^*. \quad (3.14)$$

The transformed free energy W^* for functions defined on Ω^* is, therefore, given as

$$W^*(\xi, \nabla_\xi \varphi^*(\xi)) = W(\nabla_\xi \varphi^*(\xi) \nabla_x \zeta(\zeta^{-1}(\xi))) \det[\nabla_x \zeta^{-1}]. \quad (3.15)$$

In the case that the transformation is only a rigid rotation, i.e., $\zeta(x) = \bar{Q}.x$, the former turns into

$$W^*(\nabla_\xi \varphi^*(\xi)) = W(\nabla_\xi \varphi^*(\xi) \bar{Q}). \quad (3.16)$$

Isotropy is form-invariance of W under such a transformation, thus

$$W^*(X) \stackrel{\text{isotropy}}{\widehat{=}} W(X) \quad \Rightarrow \quad \forall \bar{Q} \in \text{SO}(3) : \quad W(X\bar{Q}) = W(X). \quad (3.17)$$

In order to extent isotropy to the multiplicative decomposition, we make one preliminary assumption for illustration only: F_p is viewed formally as being a plastic gradient $\nabla \Psi_p$ with $\Psi_p : \Omega_{\text{ref}} \subset \mathbb{R}^3 \mapsto \mathbb{R}^3$. Next, the transformation of Ψ_p to a rigidly rotated configuration is obtained as

$$\Psi_p^*(\bar{Q}x) := \Psi_p(x) \quad \Rightarrow \quad \nabla_{x^*} \Psi_p^*(x^*) \bar{Q} = \nabla_x \Psi_p(x). \quad (3.18)$$

This motivates the transformation rule for F_p under a rigid transformation of the reference configuration as

$$F_p^*(x^*) = F_p^*(\bar{Q}x) = F_p(x) \bar{Q}^T. \quad (3.19)$$

Using this definition we are in a position to subsequently extend the G-covariance condition (3.9) also to include plastic gradients: for **referential isotropy we postulate the form-invariance of the energy storage terms under a rigid rotation of the coordinates**. From the transformation law, we have

$$\int_{\xi \in \Omega^*} W_{\text{ph}}(F_p^*(\xi) \bar{Q}) \det[Q^T] d\xi, \quad (3.20)$$

such that

$$W_{\text{ph}}^*(F_p^*(\xi)) := W_{\text{ph}}(F_p^*(\xi) \bar{Q}), \quad (3.21)$$

and form-invariance demands that

$$W_{\text{ph}}^*(X) = W_{\text{ph}}(X) \quad \Rightarrow \quad \forall \bar{Q} \in \text{SO}(3) : \quad W_{\text{ph}}(X\bar{Q}) = W_{\text{ph}}(X). \quad (3.22)$$

Now we can apply the same consideration of **form-invariance** to the **dislocation energy storage**. In this case, then, the transformed energy reads

$$\int_{\xi \in \Omega^*} W_{\text{curl}}(F_p^*(\xi) \bar{Q}, \text{Curl}_x[F_p^*(\xi) \bar{Q}]) \det[Q^T] d\xi, \quad (3.23)$$

such that

$$W_{\text{curl}}^*(F_p^*(\xi), \text{Curl}_\xi[F_p^*(\xi)]) := W_{\text{curl}}(F_p^*(\xi) \bar{Q}, \text{Curl}_x[F_p^*(\xi) \bar{Q}]). \quad (3.24)$$

From a lengthy calculation in indicial notation, it holds⁸

$$\text{Curl}_x[F_p^*(\bar{Q}x)\bar{Q}] = [\text{Curl}_\xi F_p^*(\xi)]\bar{Q}, \quad (3.25)$$

which leads to

$$W_{\text{curl}}^*(F_p^*(\xi), \text{Curl}_\xi[F_p^*(\xi)]) := W_{\text{curl}}(F_p^*(\xi)\bar{Q}, [\text{Curl}_\xi F_p^*(\xi)]\bar{Q}). \quad (3.26)$$

Form-invariance for the dislocation energy storage demands therefore that

$$W_{\text{curl}}^*(X, Y) = W_{\text{curl}}(X, Y) \quad \Rightarrow \quad W_{\text{curl}}(X\bar{Q}, YQ) = W_{\text{curl}}(X, Y) \quad \forall \bar{Q} \in \text{SO}(3) \quad (3.27)$$

which is satisfied for $W_{\text{curl}}(X, Y) = \|X^{-1}Y\|^2$.⁹

3.5 Rigid rotation of the material and spatial coordinates

Let the reference configuration Ω_{ref} be rigidly rotated through **one constant rotation** $Q_2 \in \text{SO}(3)$. We let $\Omega_{\text{ref}}^* = Q_2 \cdot \Omega_{\text{ref}}$ together with the rotated coordinates $x^* = Q_2 \cdot x$. Assume also that the spatial coordinate system is rigidly rotated by Q_1 . The deformation w.r.t. the rotated coordinate systems is denoted by $\varphi^*(x^*)$. It holds

$$\varphi^*(x^*) = Q_1 \varphi(x) \quad \text{i.e.} \quad \Leftrightarrow \quad \varphi^*(Q_2 \cdot x) = Q_1 \cdot \varphi(x), \quad \forall x \in \Omega_{\text{ref}}, \quad (3.28)$$

whether or not the material response is isotropic.¹⁰ From (3.28) we obtain from the chain rule

$$\begin{aligned} \nabla_x[\varphi^*(x^*)] &= \nabla_x[Q_1 \varphi(x)] \Leftrightarrow \nabla_x[\varphi^*(Q_2 \cdot x)] = Q_1 \nabla_x \varphi(x) \Leftrightarrow \nabla_{x^*}[\varphi^*(x^*)] Q_2 = Q_1 \nabla_x \varphi(x) \\ Q_1^T \nabla_{x^*}[\varphi^*(x^*)] Q_2 &= \nabla_x \varphi(x). \end{aligned} \quad (3.29)$$

The rotated free energy is denoted by $W^*(F^*)$ with $F^* = \nabla_{x^*}[\varphi^*(x^*)]$. It must be defined such that **the "rotated" minimization problem based on $W^*(F^*)$ furnishes the rotated solution** and that the energy of the materially and spatially rotated solution is equal to the energy of the unrotated solution. Thus

$$\begin{aligned} W^*(F^*) &= W^*(\nabla_{x^*} \varphi^*(x^*)) = W^*(Q_1 \nabla_x \varphi(x) Q_2^T) := W(\nabla_x \varphi(x)) \Rightarrow \\ W^*(F^*) &= W(Q_1^T F^* Q_2). \end{aligned} \quad (3.30)$$

⁸The (1,1)-component in the matrix from the left hand side of (3.25) is equal to

$$\frac{\partial}{\partial x_2} (F_p^*)_k^1(\bar{Q}x) \bar{Q}_3^k - \frac{\partial}{\partial x_3} (F_p^*)_k^1(\bar{Q}x) \bar{Q}_2^k = \frac{\partial}{\partial \xi_l} (F_p^*)_k^1(\xi) [\bar{Q}_2^l \bar{Q}_3^k - \bar{Q}_3^l \bar{Q}_2^k].$$

By orthogonality of the matrix \bar{Q} we obtain that the (1,1)-component is equal to

$$\left[\frac{\partial}{\partial \xi_2} (F_p^*)_3^1(\xi) - \frac{\partial}{\partial \xi_3} (F_p^*)_2^1(\xi) \right] \bar{Q}_1^1 + \left[\frac{\partial}{\partial \xi_3} (F_p^*)_1^1(\xi) - \frac{\partial}{\partial \xi_1} (F_p^*)_3^1(\xi) \right] \bar{Q}_2^1 + \left[\frac{\partial}{\partial \xi_1} (F_p^*)_2^1(\xi) - \frac{\partial}{\partial \xi_2} (F_p^*)_1^1(\xi) \right] \bar{Q}_3^1,$$

which is the (1,1)-component of the matrix from the right hand side of (3.25). The proof for the other components is similar.

⁹Also satisfied for $\|Y X^T\|^2$ leading to a dislocation energy storage of the form $\|[\text{Curl} F_p(x)] F_p^T(x)\|^2$, cf. (3.42).

¹⁰For isotropy, the reference configuration (the referential coordinate system) is rotated but the spatial system is not; nevertheless, if the material is isotropic, the resulting response is the same.

This identity is used to define the rotated energy. **If W happens to be objective and isotropic, i.e., form-invariant w.r.t. left and right multiplication by (not necessarily equal) constant rotation matrices (material and spatial covariance),** then $W(Q_1^T X Q_2) = W(X)$ and from (3.30) follows

$$W^*(X) = W(X). \quad (3.31)$$

We now repeat the rigid rotations for each function appearing in (3.6) separately, i.e., it follows

$$\begin{aligned} \Psi_p^*(Q_2^p \cdot x) = Q_3^p \Psi_p(x) &\Rightarrow Q_3^{p,T} \nabla_{x^*} [\Psi_p^*(x^*)] Q_2^p = \nabla_x \Psi_p(x), \\ \Psi_e^*(Q_3^e \cdot \eta) = Q_1^e \Psi_e(\eta) &\Rightarrow Q_1^{e,T} \nabla_{\eta^*} [\Psi_e^*(\eta^*)] Q_3^e = \nabla_\eta \Psi_e(\eta), \\ \varphi^*(Q_2 \cdot x) = Q_1 \varphi(x) &\Rightarrow Q_1^T \nabla_{x^*} [\varphi^*(x^*)] Q_2 = \nabla_x \varphi(x). \end{aligned} \quad (3.32)$$

By choosing $Q_1 = Q_1^e$, $Q_2 = Q_2^p$, $Q_3 = Q_3^p$ we observe that the composition of mappings carries over

$$\begin{aligned} \varphi^*(x^*) &= Q_1 \varphi(x) = Q_1 \Psi_e(\Psi_p(x)) = Q_1 \Psi_e(Q_3^T \Psi_p^*(x^*)) \\ &= Q_1 [Q_1^T \Psi_e^*(Q_3 [Q_3^T \Psi_p^*(x^*)])] = \Psi_e^*(\Psi_p^*(x^*)), \end{aligned} \quad (3.33)$$

which implies

$$\nabla_{x^*} \varphi^*(x^*) = \nabla_{\eta^*} \Psi_e^*(\Psi_p^*(x^*)) \nabla_{x^*} \Psi_p^*(x^*), \quad F^*(x^*) = F_e^*(\eta^*) F_p^*(x^*). \quad (3.34)$$

This lets us identify

$$F_e^*(\eta^*) = \nabla_{\eta^*} \Psi_e^*(\Psi_p^*(x^*)), \quad F_p^*(x^*) = \nabla_{x^*} \Psi_p^*(x^*). \quad (3.35)$$

However,

$$\begin{aligned} Q_1 \nabla \varphi(x) Q_2^T &= Q_1 \nabla_\eta \Psi_e(\Psi_p(x)) \nabla_x \Psi_p(x) Q_2^T = Q_1 \nabla_\eta \Psi_e(\Psi_p(x)) Q_3^T Q_3 \nabla_x \Psi_p(x) Q_2^T \\ Q_1 F(x) Q_2^T &= Q_1 F_e(x) Q_3^T (Q_3 F_p(x) Q_2^T) = Q_1 F_e(x) F_p(x) Q_3^T, \end{aligned} \quad (3.36)$$

but $F(x) = F_e(x) F_p(x)$ implies

$$\underbrace{Q_1 F(x) Q_2^T}_{=F^*(x^*)} = Q_1 F_e(x) Q_3^T Q_3 F_p(x) Q_2^T = \underbrace{Q_1 F_e(x) Q_3^T}_{=:F_e^*(\eta^*)} \underbrace{(Q_3 F_p(x) Q_2^T)}_{=F_p^*(x^*)}, \quad (3.37)$$

which shows, how the rotated elastic deformation gradient F_e^* must be related to the unrotated elastic deformation gradient F_e under rotations of the reference, intermediate and spatial coordinates. In fact the former equation is used as a definition of F_e^* in terms of F_e under rotation of the intermediate and spatial configuration.

Hence it is shown that under a rigid rotation of the reference configuration and simultaneous rotation of the intermediate and spatial coordinates the following obtains

$$\begin{aligned} F^*(x^*) &= Q_2 F(x) Q_1^T, \quad F_e^*(\eta^*) = Q_1 F_e(\eta) Q_3^T, \\ F_p^*(x^*) &= Q_3 F_p(x) Q_1^T = Q_3 F_p(Q_2^T x^*) Q_1^T. \end{aligned} \quad (3.38)$$

Since such changes of coordinates leave the composition of mappings invariant we require that our model be form-invariant under these transformations. We refer to this as **full elasto-plastic transformation covariance requirement**.¹¹ Note that the postulated transformation law (3.38) for the multiplicative decomposition is not meant to read:

$$\begin{aligned} F(x) = F_e(x)F_p(x) &\Rightarrow Q_1(x)F(x)Q_2(x)^T = Q_1(x)F_e(x)Q_3^T(x)Q_3(x)F_p(x)Q_2(x)^T \Rightarrow \\ F(x) = F_e(x)Q_3^T(x)Q_3(x)F_p(x) &= F_e^*(x)F_p^*(x), \end{aligned} \quad (3.39)$$

for all non-constant rotations $Q_{1,2,3}(x) \in \text{SO}(3)$. Requiring (3.39) would reduce the theory necessarily to a model based only on the plastic metric $C_p(x) = F_p^T(x)F_p(x)$. The much more restrictive condition (3.39) is sometimes motivated by the observation that the multiplicative split is locally unique only up to a local rotation $Q_3(x) \in \text{SO}(3)$, which, viewed without compatibility requirements, is self-evident. It has already been observed by Casey/Naghdi [5, (13)] that full local objectivity-requirements on the multiplicative decomposition (allow non-constant matrices in (3.38)) reduces the model to an isotropic formulation in $C = F^T F$ and $C_p = F_p^T F_p$. Our development shows that this conclusion is strictly constraint to the local theory without plastic strain gradients.

For a fully rotationally covariant model the covariant transformation behaviour of the elastic energy (3.31) under (3.38) will be postulated for all contributions separately, i.e., for all constant $Q_{1,2,3} \in \text{SO}(3)$ it must be satisfied

$$\begin{aligned} W_e^*(X) &:= W_e(Q_1^T X Q_3) = W_e(X), \\ W_{\text{ph}}^*(X) &:= W_{\text{ph}}(Q_3^T X Q_2) = W_{\text{ph}}(X), \\ W_{\text{curl}}^*(X, \text{Curl}_{x^*} X) &:= W_{\text{curl}}(Q_3^T X Q_2, \text{Curl}_x [Q_3^T X Q_2]) \\ &= W_{\text{curl}}(Q_3^T X Q_2, Q_3^T [\text{Curl}_\xi X] Q_2) = W_{\text{curl}}(X, \text{Curl}_\xi X), \\ W_{\text{curl}}(Q_3^T X Q_2, Q_3^T Y Q_2) &= W_{\text{curl}}(X, Y). \end{aligned} \quad (3.40)$$

Thus W_e and W_{ph} must be isotropic and objective functions of their arguments which is easily met whenever the functional dependence can be reduced to isotropic functions of $C_e = F_e^T F_e$ and $C_p = F_p^T F_p$.

3.6 The finite strain thermodynamic potential

Henceforth we postulate the invariance of the plasticity model according to (3.38) and (3.31). Let us start with writing down a modified Saint-Venant Kirchhoff¹² isotropic quadratic energy W_e in the elastic stretches $F_e^T F_e$, augmented with local self-hardening

¹¹It should be noted that in the case of the parametrization of shells with a planar reference configuration, the compatible F_p introduces nothing else than a stress free reference configuration.

¹²For our purpose, the Saint-Venant energy is sufficient although it is not Legendre-Hadamard elliptic at given F_p . The Saint-Venant Kirchhoff is certainly useful for small elastic strains and large displacement as is the case in finite-plasticity.

W_{ph} and a contribution accounting for plastic gradients W_{curl}

$$W(F_e, F_p, \text{Curl } F_p) = W_e(F_e) + W_{\text{ph}}(F_p) + W_{\text{curl}}(F_p, \text{Curl } F_p), \quad (3.41)$$

$$W_e(F_e) = \frac{\mu}{4} \left\| \frac{F_e^T F_e}{\det[F_e]^{2/3}} - \mathbb{1} \right\|^2 + \frac{\lambda}{4} \left((\det[F_e] - 1)^2 + \left(\frac{1}{\det[F_e]} - 1 \right)^2 \right),$$

$$W_{\text{ph}}(F_p) = \frac{\mu h^+}{4} \left\| \frac{F_p^T F_p}{\det[F_p]^{2/3}} - \mathbb{1} \right\|^2, \quad W_{\text{curl}}(F_p^{-1}, \text{Curl } F_p) = \frac{\mu L_c^2}{2} \|F_p^{-1} \text{Curl } F_p\|^2.$$

Note that here F_p is not needed to be volume preserving. Here, μ, λ are the classical isotropic Lamé-parameters, h^+ is the dimensionless hardening modulus, L_c is the internal plastic length. This energy is materially and spatially covariant and satisfies the plastic indifference condition. The elastic energy W_e is additively decoupled into a volumetric and isochoric contribution, it is objective and isotropic w.r.t. the intermediate configuration. The term W_{ph} accounts for **phenomenological local plastic hardening** in the spirit of Prager constant linear hardening, cf.(4.13). It is fully covariant and indifferent to plastic volume changes. The term W_{curl} represents energy storage due to dislocations. The argument $G_{\text{R}} = F_p^{-1} \text{Curl } F_p$ is the referential version of the tensor $G = \frac{1}{\det[F_p]} (\text{Curl } F_p) F_p^T$, called the **geometric dislocation density tensor** in the intermediate configuration. G represents the incompatibility of the intermediate configuration F_p relative to the associated surface elements. The tensor G has the virtue to be form-invariant under compatible changes in the reference configuration [48, 15, 6, 51]. It transforms as $G(QF_p) = QG(F_p)Q^T$ for all rigid rotations Q . This tensor introduces the influence of **geometrically (kinematically) necessary dislocations** (GND's). In Gurtins notation this is G^T , and he refers to this tensor as the **local Burgers tensor in the lattice configuration** measured per unit surface area in this configuration. As such it corresponds "conceptually" to an objective tensor in the "actual" configuration, like the finite strain Cauchy stress tensor σ , which satisfies as well the invariances $\forall Q \in \text{SO}(3) : \sigma(QF) = Q\sigma(F)Q^T$. Note that our corresponding referential measure G_{R} [15, Eq.(6.1)] is given by

$$G_{\text{R}} = F_p^{-1} \text{Curl } F_p, \quad G = \frac{1}{\det[F_p]} (\text{Curl } F_p) F_p^T = \frac{1}{\det[F_p]} F_p G_{\text{R}} F_p^T. \quad (3.42)$$

The referential measure G_{R} is easily seen to be invariant under a compatibel (homogeneous) change of the intermediate configuration, i.e.,

$$F(x) = F_e(x) F_p(x) = F_e(x) \bar{B}^{-1} \bar{B} F_p(x) = \tilde{F}_e(x) \tilde{F}_p(x),$$

$$G_{\text{R}}(\bar{B} F_p(x)) = G_{\text{R}}(F_p(x)), \quad \forall \bar{B} \in \text{GL}^+(3), \quad (3.43)$$

while the local plastic self-hardening would be invariant under $F_p \mapsto \mathbb{R}^+ \text{SO}(3) \cdot F_p$ only.

3.7 Derivation of the finite strain evolution equations

Having postulated as thermodynamic potential (3.41) it remains to motivate the flow rule. thermodynamic driving forces. Relevant in this respect are the thermodynamical driving

forces acting on the internal variable F_p . Therefore, locally in a space point $x \in \Omega$

$$\begin{aligned}
\frac{d}{dt} W_e(F(t_0), F_p^{-1}(t)) &= \langle DW_e(F F_p^{-1}), F \frac{d}{dt} F_p^{-1} \rangle = \langle DW_e(F_e), F F_p^{-1} F_p \frac{d}{dt} F_p^{-1} \rangle \\
&= \langle F_e^T DW_e(F_e), F_p \frac{d}{dt} F_p^{-1} \rangle = \langle \Sigma_e, F_p \frac{d}{dt} F_p^{-1} \rangle, \\
\langle DW_{\text{ph}}(F_p), \frac{d}{dt} F_p \rangle &= \langle DW_{\text{ph}}(F_p), [\frac{d}{dt} F_p] F_p^{-1} F_p \rangle = \langle DW_{\text{ph}}(F_p) F_p^T, \frac{d}{dt} F_p F_p^{-1} \rangle \\
&= \langle -DW_{\text{ph}}(F_p), F_p \frac{d}{dt} F_p^{-1} \rangle = \langle \Sigma_{\text{sh}}, F_p \frac{d}{dt} F_p^{-1} \rangle. \tag{3.44}
\end{aligned}$$

For the nonlocal term, the product $\langle A, B \rangle$ includes also integration over the domain Ω and we will use the self-adjointness of the Curl-operator provided the boundary conditions are suitably chosen, i.e., at least the appropriate **insulation condition**¹³ does hold. Then

$$\begin{aligned}
&\langle DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p), F_p^{-1} \text{Curl } \frac{d}{dt} F_p + \frac{d}{dt} F_p^{-1} \text{Curl } F_p \rangle \\
&= \langle \text{Curl}(F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p)), \frac{d}{dt} F_p \rangle + \langle DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p) (\text{Curl } F_p)^T, \frac{d}{dt} F_p^{-1} \rangle \\
&= \langle \text{Curl}(F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p) F_p^T, -F_p \frac{d}{dt} F_p^{-1} \rangle \\
&\quad + \langle F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p) (\text{Curl } F_p)^T, F_p \frac{d}{dt} F_p^{-1} \rangle = \langle \Sigma_{\text{curl}}, F_p \frac{d}{dt} F_p^{-1} \rangle. \tag{3.46}
\end{aligned}$$

Let us also define the elastic domain in stress-space $\mathcal{E} := \{\Sigma \in \mathbb{M}^{3 \times 3} \mid \|\text{dev } \Sigma\| \leq \sigma_y\}$, with yield stress σ_y , corresponding indicator function

$$\chi(\Sigma) = \begin{cases} 0 & \|\text{dev } \Sigma\| \leq \sigma_y \\ \infty & \text{else,} \end{cases} \tag{3.47}$$

¹³In the finite-strain case the **insulation condition** reads

$$\begin{aligned}
&\int_{\Omega} \underbrace{\langle F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p), \text{Curl}[\frac{d}{dt} F_p] \rangle}_{\hat{\Sigma}} dV \\
&= \int_{\Omega} \langle \text{Curl}[F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl } F_p)], \frac{d}{dt} F_p \rangle dV + \underbrace{\int_{\partial\Omega} \langle \hat{\Sigma} \times \frac{d}{dt} F_p, \vec{N} \rangle dS}_{\text{insulation condition } = 0}, \tag{3.45}
\end{aligned}$$

and can be satisfied, if, e.g., $F_p(x, t) \cdot \tau = F_p(x, 0) \cdot \tau$ on $x \in \Gamma_D$ (implies $\frac{d}{dt} F_p \cdot \tau = 0$ there) and $\text{Curl } F_p \cdot \tau = 0$ on $\partial\Omega \setminus \Gamma_D$.

and subdifferential in the sense of convex analysis ¹⁴

$$\partial\mathcal{X}(\Sigma) = \begin{cases} 0 & \|\operatorname{dev} \Sigma\| < \sigma_y \\ \mathbb{R}_0^+ \frac{\operatorname{dev} \Sigma}{\|\operatorname{dev} \Sigma\|} & \|\operatorname{dev} \Sigma\| = \sigma_y \\ \emptyset & \|\operatorname{dev} \Sigma\| > \sigma_y . \end{cases} \quad (3.50)$$

Note that **choosing** $\operatorname{dev} \Sigma$ **instead of** $\operatorname{dev} \operatorname{sym} \Sigma$ **in** (3.47) **allows for plastic spin**. Putting together the associative flow rule the finite strain model in a classical formulation reads: find

$$\begin{aligned} \varphi &\in C^1([0, T]; C^1(\bar{\Omega}, \mathbb{R}^3)), & F_p &\in C^1([0, T]; C(\bar{\Omega}, \operatorname{SL}(3))), \\ \operatorname{Curl} F_p(t) &\in L^2(\Omega, \mathbb{M}^{3 \times 3}), & \Sigma_{\operatorname{curl}}(t) &\in L^2(\Omega, \mathbb{M}^{3 \times 3}), \end{aligned} \quad (3.51)$$

such that

$$\begin{aligned} \operatorname{Div} S_1(F_e) &= -f, & S_1(F_e) &= D_F[W_e(F F_p^{-1})] = DW_e(F_e) \cdot F_p^{-T}, \\ F_p \frac{d}{dt}[F_p^{-1}] &\in -\partial\mathcal{X}(\Sigma), & \Sigma &= \Sigma_e + \Sigma_{\operatorname{sh}} + \Sigma_{\operatorname{curl}}, \\ \Sigma_e &= F_e^T DW_e(F_e), & \Sigma_{\operatorname{sh}} &= -DW_{\operatorname{ph}}(F_p) F_p^T, \\ \Sigma_{\operatorname{curl}} &= F_p^{-T} DW_{\operatorname{curl}}(F_p^{-1} \operatorname{Curl} F_p) (\operatorname{Curl} F_p)^T - \operatorname{Curl} (F_p^{-T} DW_{\operatorname{curl}}(F_p^{-1} \operatorname{Curl} F_p)) F_p^T, \\ \varphi(x, t) &= g_d(x, t), & F_p(x, t) \cdot \tau &= F_p(x, 0) \cdot \tau, \quad x \in \Gamma_D, \\ 0 &= [\operatorname{Curl} F_p(x, t)] \cdot \tau, & x \in \partial\Omega \setminus \Gamma_D, & F_p(x, 0) = F_p^0(x). \end{aligned} \quad (3.52)$$

Note that the **local contributions are fully rotationally invariant (isotropic and objective)** with respect to the transformation

$$\forall Q_{1,2,3} \in \operatorname{SO}(3) : (F, F_e, F_p) \mapsto (Q_1(x) F Q_2(x)^T, Q_1(x) F_e Q_3(x)^T, Q_3(x) F_p Q_2(x)^T), \quad (3.53)$$

and the nonlocal dislocation potential is still invariant with respect to the corresponding rigid transformation

$$\forall \bar{Q}_{1,2,3} \in \operatorname{SO}(3) : (F, F_e, F_p) \mapsto (\bar{Q}_1 F \bar{Q}_2^T, \bar{Q}_1 F_e \bar{Q}_3^T, \bar{Q}_3 F_p \bar{Q}_2^T). \quad (3.54)$$

¹⁴The subdifferential for a convex function $\mathcal{X} : \mathbb{M}^{3 \times 3} \mapsto \mathbb{R}^+$ is defined as $\partial\mathcal{X}(\Sigma) = \emptyset$ for $\Sigma : \mathcal{X}(\Sigma) = \infty$ and otherwise through

$$\zeta \in \partial\mathcal{X}(\Sigma) \Leftrightarrow \forall H \in \mathbb{M}^{3 \times 3} : \mathcal{X}(\Sigma + H) \geq \mathcal{X}(\Sigma) + \langle \zeta, H \rangle. \quad (3.48)$$

Note that whenever $\Sigma + H \notin \mathcal{E}$ then $\mathcal{X}(\Sigma + H) = \infty$ and the last inequality generates no constraint on ζ . Therefore we have the equivalent characterization

$$\zeta \in \partial\mathcal{X}(\Sigma) \Leftrightarrow \forall H \in \mathfrak{sl}(3) : \mathcal{X}(\Sigma + H) \geq \mathcal{X}(\Sigma) + \langle \zeta, H \rangle. \quad (3.49)$$

Since W_e and W_{ph} satisfy $W_e(Q(x)F_e)Q(x)^T = W_e(F_e)$ and $W_{\text{ph}}(Q(x)F_p)Q(x)^T = W_{\text{ph}}(F_p)$ the following statements are automatically true:

$$\begin{aligned}\Sigma_e(Q(x)F_eQ(x)^T) &= Q(x)\Sigma_e(F_e)Q(x)^T, \quad \Sigma_e \in \text{Sym}(3), \\ \Sigma_{\text{sh}}(Q(x)F_pQ(x)^T) &= Q(x)\Sigma_{\text{sh}}(F_p)Q(x)^T, \quad \Sigma_{\text{sh}} \in \text{Sym}(3), \\ \Sigma_{\text{curl}}(\overline{Q}F_p \text{Curl}[\overline{Q}F_p]) &= \overline{Q}\Sigma_{\text{curl}}(F_p, \text{Curl} F_p)\overline{Q}^T, \quad \overline{Q} = \text{const.}, \\ \Sigma_{\text{curl}}(\overline{Q}^T X \overline{Q}, \overline{Q}^T Y \overline{Q}) &= \overline{Q}^T \Sigma_{\text{curl}}(X, Y)\overline{Q}, \quad \overline{Q} = \text{const.},\end{aligned}\tag{3.55}$$

In general, Σ_{curl} is **not symmetric**, thus, the plastic inhomogeneity is responsible for the plastic spin contribution in this covariant formulation. Since $\partial\mathcal{X}$ is monotone, the formulation is thermodynamically admissible. This remains true if we replace $\partial\mathcal{X}$ with a general flow function $\mathfrak{f} : \mathbb{M}^{3 \times 3} \mapsto \mathbb{M}^{3 \times 3}$ which is only pre-monotone.

3.8 Reformulation of the finite strain problem

Using the Legendre-transformation of the flow potential one can equivalently rewrite the flow rule

$$\begin{aligned}F_p \frac{d}{dt}[F_p^{-1}] \in -\partial\mathcal{X}(\Sigma) &\Leftrightarrow \Sigma \in \partial\mathcal{X}^*(-F_p \frac{d}{dt}[F_p^{-1}]) \Leftrightarrow \\ \mathcal{X}^*(q) - \mathcal{X}^*(-F_p \frac{d}{dt}[F_p^{-1}]) &\geq \langle \Sigma, q - [-F_p \frac{d}{dt}[F_p^{-1}]] \rangle \quad \forall q \in \mathfrak{sl}(3).\end{aligned}\tag{3.56}$$

Inserting the constitutive relation for Σ , integrating over the domain Ω and partial integration (using the conditions leading to the insulation condition (3.45)), shows that it must hold

$$\begin{aligned}\int_{\Omega} \mathcal{X}^*(q(t, x)) - \mathcal{X}^*(-F_p \frac{d}{dt}[F_p^{-1}]) dV &\geq \int_{\Omega} \langle \Sigma_e + \Sigma_{\text{sh}} + \Sigma_{\text{dis}}^1, q + F_p \frac{d}{dt}[F_p^{-1}] \rangle \\ &- \langle \Sigma_{\text{dis}}^2, \text{Curl}[q + F_p \frac{d}{dt}[F_p^{-1}]F_p] \rangle dV \quad \forall q \in L^2(0, T; H_{\text{curl}}(\Omega, \mathfrak{sl}(3))), \\ \Sigma_{\text{curl}} &= \Sigma_{\text{dis}}^1 - (\text{Curl} \Sigma_{\text{dis}}^2) F_p^T, \quad \Sigma_{\text{dis}}^1 = F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl} F_p) (\text{Curl} F_p)^T, \\ \Sigma_{\text{dis}}^2 &= (F_p^{-T} DW_{\text{curl}}(F_p^{-1} \text{Curl} F_p)).\end{aligned}\tag{3.57}$$

Hence, solutions of (3.52) satisfy as well

$$\begin{aligned}0 &= \int_{\Omega} \langle S_1(F_e), \nabla \xi \rangle - \langle f, \xi \rangle dV \quad \forall \xi \in H^1(\Omega, \mathbb{R}^3), \\ S_1(F_e) &= D_F[W_e(F F_p^{-1})] = DW_e(F_e) \cdot F_p^{-T}, \\ 0 &\leq \int_{\Omega} \mathcal{X}^*(q(t, x)) - \mathcal{X}^*(-F_p \frac{d}{dt}[F_p^{-1}]) - \langle \Sigma_e + \Sigma_{\text{sh}} + \Sigma_{\text{dis}}^1, q + F_p \frac{d}{dt}[F_p^{-1}] \rangle \\ &+ \langle \Sigma_{\text{dis}}^2, \text{Curl}[q + F_p \frac{d}{dt}[F_p^{-1}]F_p] \rangle dV \quad \forall q \in L^2(0, T; H_{\text{curl}}(\Omega, \mathfrak{sl}(3))),\end{aligned}$$

$$\varphi(x, t) = g_d(x, t), \quad F_p(x, t) \cdot \tau = F_p(x, 0) \cdot \tau, \quad x \in \Gamma_D, \quad F_p(x, 0) = F_p^0(x).$$

Adding (4.1)₁ and (4.1)₂ yields a mixed variational inequality which is automatically satisfied by solutions of (3.52).

4 The geometrically linear gradient plasticity model

The corresponding linearized model can either be obtained by linearizing all quantities, e.g., replacing $\Sigma_e \mapsto \text{Lin}(\Sigma_e) = \sigma$ or, more elegantly by writing down the corresponding quadratic potential in linearized quantities. Thus we expand $F = \mathbb{1} + \nabla u$, $F_p = \mathbb{1} + p + \dots$, $F_e = \mathbb{1} + e + \dots$ and the multiplicative decomposition (3.1) turns into

$$\begin{aligned} \mathbb{1} + \nabla u &= (\mathbb{1} + e + \dots)(\mathbb{1} + p + \dots) \rightsquigarrow \nabla u \approx e + p + \dots, \\ F_e^T F_e - \mathbb{1} &= \mathbb{1} + 2 \text{sym } e + e^T e - \mathbb{1} \rightsquigarrow 2 \text{sym } e = 2 \text{sym}(\nabla u - p). \end{aligned} \quad (4.1)$$

Hence one obtains to highest order the **additive decomposition** [21, 23] of the displacement gradient $\nabla u = e + p$, with $\text{sym } e = \text{sym}(\nabla u - p)$ the **infinitesimal elastic lattice strain**, skew $e = \text{skew}(\nabla u - p)$ the **infinitesimal elastic lattice rotation** and $\kappa_e = \nabla \text{axl}(\text{skew } e)$ the **infinitesimal elastic lattice curvature** [30] and p the **infinitesimal plastic distortion**. The quadratic energy which corresponds to (3.41) is given by

$$\begin{aligned} W(\nabla u, p, \text{Curl } p) &= W_e^{\text{lin}}(\nabla u - p) + W_{\text{ph}}(p) + W_{\text{curl}}^{\text{lin}}(\text{Curl } p), \\ W_e^{\text{lin}}(\nabla u - p) &= \mu \|\text{sym}(\nabla u - p)\|^2 + \frac{\lambda}{2} \text{tr}[\nabla u - p]^2, \\ W_{\text{ph}}^{\text{lin}}(p) &= \mu h^+ \|\text{dev sym } p\|^2, \quad W_{\text{curl}}^{\text{lin}}(\text{Curl } p) = \frac{\mu L_c^2}{2} \|\text{Curl } p\|^2. \end{aligned} \quad (4.2)$$

The used free energy coincides with that in [30, p. 1783] apart for our local kinematical hardening contribution. Note that the **infinitesimal plastic distortion** $p : \Omega \subset \mathbb{R}^3 \mapsto \mathbb{M}^{3 \times 3}$ need **not be symmetric**, but that only its symmetric part, the **infinitesimal plastic strain**¹⁵ $\text{sym } p$, contributes to the local elastic energy expression. The **infinitesimal plastic rotation** skew p does not locally contribute to the elastic energy neither contributes to the local plastic self-hardening but appears in the nonlocal hardening. The resulting elastic energy is invariant under infinitesimal rigid rotations $\nabla u \mapsto \nabla u + \bar{A}$, $\bar{A} \in \mathfrak{so}(3)$ of the body. The invariance of the curvature contribution needs the homogeneity of the rotations.¹⁶

Provided that the infinitesimal plastic distortion p is known, (4.2) defines a linear elasticity problem with pre-stress for the displacement u . It remains to provide an evolution law for p which is consistent with thermodynamics. To this end we use a nonlocal

¹⁵The notation $\varepsilon_p \in \text{Sym}(3)$ is strictly reserved to the purely local theory.

¹⁶Note that it is the frame-indifference w.r.t. F_e that leaves us finally with the infinitesimal elastic lattice strain measure $\text{sym}(\nabla u - p)$. If we would consider instead a purely macroscopic formulation based on an **evolving symmetric plastic metric** $C_p = F_p^T F_p$ (Casey/Naghdi [38]) with corresponding elastic strain measure $E = C - C_p$, then, upon linearization, we would arrive as well at $\text{sym}(\nabla u - p)$ but the model would feature **only** a symmetric plastic strain $\varepsilon_p := \text{sym } p$ ($C_p = F_p^T F_p$ is invariant w.r.t. $F_p \mapsto Q F_p$ and $\text{sym } p$ is invariant w.r.t. $p \mapsto p + A$ for $A \in \mathfrak{so}(3)$). Including a higher plastic gradient based on C_p would require the introduction of a compatibility measure for C_p of the form $\mathcal{R}(C_p) = 0 \Rightarrow \exists \psi_p : \Omega \mapsto \mathbb{R}^3 : C_p = \nabla \Psi_p^T \nabla \Psi_p$. The corresponding operator \mathcal{R} is a second order differential operator. Linearizing the relations leads to $\text{inc}(\varepsilon_p) = 0 \Rightarrow \exists u_p : \Omega \mapsto \mathbb{R}^3 : \varepsilon_p = \text{sym } \nabla u_p$ for some displacement u_p . Here, the operator inc is the second order compatibility measure of de Saint-Venant [14, p.40] with the property $\text{inc}(\text{sym } \nabla u) = 0$ and $\text{Div inc} = 0$. Remaining in such a theory would lead to a fourth order evolution equation for ε_p , which is numerically preventive. In fact $\text{inc} = \text{curl curl}$ represents six second order conditions on ε_p .

(integral) version of the second law of thermodynamics.

For any "nice" subdomain $\mathcal{V} \subseteq \Omega$ consider for fixed $t_0 \in \mathbb{R}$

$$\begin{aligned}
& \frac{d}{dt} \int_{\mathcal{V}} W(\nabla u(x, t_0), p(x, t), \text{Curl } p(x, t)) \, dV = \\
& \int_{\mathcal{V}} 2\mu \langle \text{sym}(\nabla u - p), -\frac{d}{dt} p \rangle + \lambda \text{tr} [\text{sym}(\nabla u - p)] \text{tr} \left[-\frac{d}{dt} p \right] \\
& \quad + 2\mu h^+ \langle \text{dev sym } p, \text{dev sym } \frac{d}{dt} p \rangle + \mu L_c^2 \langle \text{Curl } p, \text{Curl } \frac{d}{dt} p \rangle \, dV \\
& = \int_{\mathcal{V}} 2\mu \langle \text{sym}(\nabla u - p), -\frac{d}{dt} p \rangle + \lambda \text{tr} [\text{sym}(\nabla u - p)] \langle \mathbb{1}, -\frac{d}{dt} p \rangle \\
& \quad - 2\mu h^+ \langle \text{dev sym } p, -\frac{d}{dt} p \rangle + \mu L_c^2 \langle \text{Curl } p, \text{Curl } \frac{d}{dt} p \rangle \, dV \\
& = \int_{\mathcal{V}} \langle 2\mu \text{sym}(\nabla u - p) + \lambda \text{tr} [\nabla u - p] \mathbb{1} - 2\mu h^+ \text{dev sym } p, -\frac{d}{dt} p \rangle \\
& \quad + \mu L_c^2 \langle \text{Curl}[\text{Curl } p], \frac{d}{dt} p \rangle + \underbrace{\sum_{i=1}^3 \text{Div } \mu L_c^2 \left(\frac{d}{dt} p^i \times (\text{curl } p)^i \right)}_{\text{"extra entropy flux" } q(p_t, \text{Curl } p)} \, dV.
\end{aligned} \tag{4.3}$$

Choosing constitutively as extra entropy flux

$$q^i = \mu L_c^2 \left(\frac{d}{dt} p^i \times (\text{curl } p)^i \right), \quad i = 1, 2, 3, \tag{4.4}$$

shows that the extended form of the reduced dissipation inequality at constant temperature (2.4) may be evaluated as follows

$$\begin{aligned}
0 & \geq \int_{\Omega} \frac{d}{dt} W(\nabla u(x, t_0), p(x, t), \text{Curl } p(x, t)) - \text{Div } q(p_t, \text{Curl } p) \, dV \\
& = \int_{\Omega} \langle 2\mu \text{sym}(\nabla u - p) + \lambda \text{tr} [\nabla u - p] \mathbb{1} - 2\mu h^+ \text{dev sym } p, -\frac{d}{dt} p \rangle \\
& \quad + \mu L_c^2 \langle \text{Curl}[\text{Curl } p], \frac{d}{dt} p \rangle \, dV \\
& = \int_{\Omega} \underbrace{\langle 2\mu \text{sym}(\nabla u - p) + \lambda \text{tr} [\nabla u - p] \mathbb{1} - 2\mu h^+ \text{dev sym } p - \mu L_c^2 \text{Curl}[\text{Curl } p], -\frac{d}{dt} p \rangle}_{=:\Sigma} \, dV \\
& = \int_{\Omega} \langle \sigma - 2\mu h^+ \text{dev sym } p - \mu L_c^2 \text{Curl}[\text{Curl } p], -\frac{d}{dt} p \rangle \, dV,
\end{aligned} \tag{4.5}$$

where Σ is the linearized Eshelby stress in disguise. Taking

$$\frac{d}{dt} p = \mathbf{f}(\Sigma), \tag{4.6}$$

where the function $\mathbf{f} : \mathbb{M}^{3 \times 3} \mapsto \mathbb{M}^{3 \times 3}$ with $\mathbf{f}(0) = 0$ satisfies the **monotonicity in zero condition**

$$\langle \mathbf{f}(\Sigma) - \mathbf{f}(0), \Sigma - 0 \rangle = \langle \mathbf{f}(\Sigma), \Sigma \rangle \geq 0, \tag{4.7}$$

ensures the correct sign in (4.5) (positive dissipation) and the evolution (4.6) is thermodynamically admissible. In the large scale limit $L_c = 0$ this is just the **class of pre-monotone type** defined by Alber [1]. Note that the driving term Σ has the dimension of stress. Note also that $\text{Div}(p_t \times \text{Curl } p) = 0$ for purely elastic processes $p_t \equiv 0$.

The remaining divergence term which has to be evaluated in order for (2.9) to hold is given by the **linearized insulation condition**

$$\int_{\Omega} \sum_{i=1}^3 \text{Div} \left(\frac{d}{dt} p^i \times (\text{curl } p)^i \right) dV = \int_{\partial\Omega} \sum_{i=1}^3 \left\langle \frac{d}{dt} p^i \times (\text{curl } p)^i, \vec{n} \right\rangle dS = 0. \quad (4.8)$$

The last condition is satisfied, e.g., if in each point of the boundary $\partial\Omega$ it holds

$$0 = \left\langle \frac{d}{dt} p^i \times (\text{curl } p)^i, \vec{n} \right\rangle, \quad x \in \partial\Omega, \quad i = 1, 2, 3, \quad (4.9)$$

which may be satisfied by postulating¹⁷

$$\begin{aligned} p(x, t) \cdot \tau &= p(x, 0) \cdot \tau, \quad x \in \Gamma_D \quad (\Rightarrow \frac{d}{dt} p(x, t) \cdot \tau = 0), \\ \text{Curl } p(x, t) \cdot \tau &= 0, \quad x \in \partial\Omega \setminus \Gamma_D. \end{aligned} \quad (4.10)$$

For the case of associated plasticity, as in the finite strain setting, let us choose $\mathbf{f}(\Sigma) = \partial\chi(\Sigma)$, where $\chi : \mathbb{M}^{3 \times 3}$, is the **indicator function of the elastic domain** which is also the **Legendre-transformation of the dissipation potential**.

Following Gurtin and Anand [17] on gradient plasticity: "Our goal is a theory that allows for constitutive dependencies on (the dislocation density tensor) G , but that otherwise does not depart drastically from the classical theory." Therefore, our guiding principles for the development of gradient plasticity are

- The **large scale limit** $L_c \rightarrow 0$ with **zero local hardening** $h^+ = 0$ should coincide with the classical **Prandtl-Reuss** model with deviatoric von Mises flow rule.
- The **large scale limit** $L_c \rightarrow 0$ should determine the plastic distortion to be **irrotational**, i.e., only $\varepsilon_p := \text{sym } p$ appears (zero plastic spin).
- The model for $L_c > 0$ should be **well-posed**. Existence and uniqueness should be obtained in suitable Hilbert-spaces.
- The model for $L_c > 0$ should contain **maximally second order derivatives** in the evolution law.
- The model for $L_c > 0$ should be **linearized materially and spatially covariant** and **thermodynamically consistent** (in the extended sense).

¹⁷It is not immediately obvious how a boundary condition on p at Γ_D can be posed. In Gurtin [18, 2.17] it is shown that the **microscopically hard condition** $\dot{p} \cdot \tau|_{\Gamma_D} = 0$ has a precise physical meaning: there is no flow of the Burgers vector across the boundary Γ_D .

- The model for $L_c > 0$ should be **isotropic** with respect to both, the **referential and intermediate configuration**.
- The model for $L_c > 0$ should contain **first order boundary conditions** on p only at the **hard Dirichlet boundary** $\Gamma_D \subset \partial\Omega$ for the deformation.
- The model for $L_c > 0$ may contain **second order boundary conditions** on p like $\text{Curl } p \cdot \tau = 0$ at the total external boundary $\partial\Omega$ or $\dot{p} \cdot \tau = 0$, motivated, perhaps from thermodynamics and insulation conditions.
- A long-term goal is to show well-posedness without local hardening, i.e., $h^+ \rightarrow 0$.

4.1 The strong formulation of geometrically linear gradient plasticity

The infinitesimal strain gradient plasticity model reads: find

$$\begin{aligned} u &\in H^1([0, T]; H_0^1(\Omega, \Gamma_D, \mathbb{R}^3)), \quad \text{sym } p \in H^1([0, T]; L^2(\Omega, \mathfrak{sl}(3))), \\ \text{Curl } p(t) &\in L^2(\Omega, \mathbb{M}^{3 \times 3}), \quad \text{Curl } \text{Curl } p(t) \in L^2(\Omega, \mathbb{M}^{3 \times 3}), \end{aligned} \quad (4.11)$$

such that

$$\begin{aligned} \text{Div } \sigma &= -f, \quad \sigma = 2\mu \text{sym}(\nabla u - p) + \lambda \text{tr}[\nabla u - p] \mathbb{1}, \\ \dot{p} &\in \partial\mathcal{X}(\Sigma^{\text{lin}}), \quad \Sigma^{\text{lin}} = \Sigma_e^{\text{lin}} + \Sigma_{\text{sh}}^{\text{lin}} + \Sigma_{\text{curl}}^{\text{lin}}, \\ \Sigma_e^{\text{lin}} &= 2\mu \text{sym}(\nabla u - p) + \lambda \text{tr}[\nabla u - p] \mathbb{1} = \sigma, \\ \Sigma_{\text{sh}}^{\text{lin}} &= -2\mu h^+ \text{dev } \text{sym } p, \quad \Sigma_{\text{curl}}^{\text{lin}} = -\mu L_c^2 \text{Curl}(\text{Curl } p), \\ u(x, t) &= u_d(x), \quad p(x, t) \cdot \tau = p(x, 0) \cdot \tau, \quad x \in \Gamma_D, \\ 0 &= [\text{Curl } p(x, t)] \cdot \tau, \quad x \in \partial\Omega \setminus \Gamma_D, \quad p(x, 0) = p^0(x). \end{aligned} \quad (4.12)$$

If $p^0 \in \text{Sym}(3)$, then $\Sigma_{\text{curl}}^{\text{lin}} = -\mu L_c^2 \text{inc}(\varepsilon_p)$, i.e., the plastic strain incompatibility drives the nonlocal hardening; moreover $\Sigma_{\text{curl}}^{\text{lin}}$ is **symmetric** provided p^0 is symmetric, contrary to the finite strain case. The mathematically suitable space for symmetric p is the classical space $H_{\text{curl}}(\Omega) := \{v \in L^2(\Omega), \text{Curl } v \in L^2(\Omega)\}$.

If, on the contrary, $p^0(x) \notin \text{Sym}(3)$, then the linearized model will also have a non-zero plastic spin. It is, therefore, the initial condition on the plastic variable p which determines whether our model is spin-free or not. These statements can be compared to [16] where a small-deformation isotropic gradient plasticity model is proposed with the feature that in the absence of dislocations ($\text{Curl } p = 0$) no plastic spin occurs. The same behaviour is obtained in our model.

Note that in the large scale limit $L_c \rightarrow 0$ we recover a classical elasto-plasticity model with local kinematic hardening. Observe that the term $\mu L_c^2 \text{Curl}(\text{Curl } p)$ acts as **nonlocal**

kinematical backstress and constitutes a crystallographically motivated alternative to merely phenomenologically motivated backstress tensors. The term $-2\mu h^+ \text{dev sym } p$ is a **symmetric local kinematical backstress**. The model is therefore able to represent linear kinematic hardening¹⁸ and Bauschinger-like phenomena. Moreover, the driving stress Σ is non-symmetric due to the presence of the second order gradients, while the local contribution σ , due to elastic lattice strains, remains symmetric.

Observe that the infinitesimal local contributions are fully rotationally invariant (isotropic and objective) with respect to the transformation $(\nabla u, p) \mapsto (\nabla u + A(x), p + A(x))$ and the nonlocal dislocation potential is still invariant with respect to the infinitesimal rigid transformation $(\nabla u, p) \mapsto (\nabla u + \bar{A}, p + \bar{A})$.

5 Mathematical results

5.1 Uniqueness of strong solutions

Assume that strong solutions to the model (4.12) exist. Let us show that these solutions are already unique. The aim of this paragraph is to study the influence of the different boundary conditions on the possible uniqueness. In that way it is aimed at identifying the weakest boundary condition which suffices for uniqueness. Possible boundary conditions are

$$\begin{aligned}
\text{pure micro-free : } & \text{Curl } p \cdot \tau = 0, \quad x \in \partial\Omega, \\
\text{micro-hard/free : } & \begin{cases} \text{Curl } p \cdot \tau = 0, & x \in \partial\Omega \setminus \Gamma_D & \text{micro-free} \\ \dot{p} \cdot \tau = 0, & x \in \Gamma_D & \text{micro-hard} \end{cases} \\
\text{pure micro-hard : } & \dot{p} \cdot \tau = 0, \quad x \in \partial\Omega, \\
\text{pure insulation condition : } & \int_{\partial\Omega} \sum_{i=1}^3 \langle \dot{p}^i \times (\text{curl } p)^i, \vec{n} \rangle \text{dS} = 0. \tag{5.1}
\end{aligned}$$

We note that the **pure insulation condition is not additively stable**, i.e., the difference of two solutions $p_1 - p_2$ which satisfy each individually the insulation condition need not satisfy the insulation condition. Thus the pure insulation condition is not a good candidate for establishing uniqueness.¹⁹

¹⁸Purely phenomenological Prager linear kinematic hardening is usually written as the system

$$\dot{\varepsilon}_p \in \partial\mathcal{X}(\sigma - b), \quad \dot{b} = 2\mu h^+ \dot{\varepsilon}_p, \tag{4.13}$$

with b the symmetric backstress tensor and $h^+ > 0$ the constant hardening modulus. Assuming $b(x, 0) = 2\mu h^+ \varepsilon_p(x, 0)$ and integration yields the format given in (4.12).

¹⁹For Gurtin [17] the insulation condition is motivated by imposing boundary conditions that result in a "null expenditure of microscopic power" and he immediately strengthens this statement to mean that the integrand in the insulation condition vanishes which is satisfied if, e.g.,

$$\begin{aligned}
\dot{p} \cdot \tau = 0, \quad x \in \Gamma_D & \quad \text{microscopically hard,} \\
\text{Curl } p \cdot \tau = 0, \quad x \in \partial\Omega \setminus \Gamma_D & \quad \text{microscopically free.} \tag{5.2}
\end{aligned}$$

Here we follow closely the uniqueness proof given in [1, p.32], using the a priori energy estimate and the monotonicity for the difference of two solutions. We allow in this part the generality of a monotone flow function \mathbf{f} instead of $\partial\mathcal{X}$. Assume that two strong solutions (u_1, p_2) and (u_2, p_2) exist (satisfying the same boundary and initial conditions). Insert the difference of the solutions into the total energy and consider the time derivative

$$\begin{aligned}
& \frac{d}{dt} \int_{\Omega} W(\nabla(u_1 - u_2), p_1 - p_2, \text{Curl}(p_1 - p_2)) dV \\
&= \int_{\Omega} \langle DW_e^{\text{lin}}(\nabla(u_1 - u_2), p_1 - p_2), \nabla\dot{u}_1 - \nabla\dot{u}_2 \rangle - \langle DW_e^{\text{lin}}(\nabla(u_1 - u_2), p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle \\
&\quad \langle DW_{\text{ph}}^{\text{lin}}(p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle + \langle DW_{\text{curl}}^{\text{lin}}(\text{Curl}(p_1 - p_2)), \text{Curl} \frac{d}{dt}(p_1 - p_2) \rangle dV \\
&= \int_{\Omega} \langle \sigma(\nabla(u_1 - u_2), p_1 - p_2), \nabla\dot{u}_1 - \nabla\dot{u}_2 \rangle - \langle \sigma(\nabla(u_1 - u_2), p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle \\
&\quad + \langle 2\mu h^+ \text{dev sym}(p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle + \langle \mu L_c^2 \text{Curl}(p_1 - p_2), \text{Curl} \frac{d}{dt}(p_1 - p_2) \rangle dV \\
&= - \int_{\Omega} \langle \text{Div} \sigma(\nabla(u_1 - u_2), p_1 - p_2), \dot{u}_1 - \dot{u}_2 \rangle dV + \int_{\partial\Omega} \langle \sigma(\nabla(u_1 - u_2), p_1 - p_2) \cdot \vec{n}, (u_1 - u_2)_t \rangle dS \\
&\quad - \langle \sigma(\nabla(u_1 - u_2), p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle + \int_{\Omega} \langle 2\mu h^+ \text{dev sym}(p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle \\
&\quad + \langle \mu L_c^2 \text{Curl}(p_1 - p_2), \text{Curl} \frac{d}{dt}(p_1 - p_2) \rangle dV \\
&= -0 + 0 + \int_{\Omega} \langle 2\mu h^+ \text{dev sym}(p_1 - p_2), \dot{p}_1 - \dot{p}_2 \rangle - \langle \sigma(\nabla(u_1 - u_2), p_1 - p_2), \nabla\dot{p}_1 - \nabla\dot{p}_2 \rangle \\
&\quad + \langle \mu L_c^2 \text{Curl} \text{Curl}(p_1 - p_2), \frac{d}{dt}(p_1 - p_2) \rangle dV \\
&= \int_{\Omega} \langle \Sigma_2^{\text{lin}} - \Sigma_1^{\text{lin}}, \dot{p}_1 - \dot{p}_2 \rangle dV = - \int_{\Omega} \langle \Sigma_2^{\text{lin}} - \Sigma_1^{\text{lin}}, \dot{p}_1 - \dot{p}_2 \rangle dV \leq 0. \tag{5.3}
\end{aligned}$$

Hence, also for the difference of two solutions,

$$\begin{aligned}
& \int_{\Omega} W(\nabla(u_1 - u_2)(t), (p_1 - p_2)(t), \text{Curl}(p_1 - p_2)(t)) dV \\
&\leq \int_{\Omega} W(\nabla(u_1 - u_2)(0), (p_1 - p_2)(0), \text{Curl}(p_1 - p_2)(0)) dV = 0. \tag{5.4}
\end{aligned}$$

Thus we have

$$\begin{aligned}
& \int_{\Omega} \|\text{sym}(\nabla(u_1 - u_2)(t) - (p_1 - p_2)(t))\|^2 dV = 0, \quad \int_{\Omega} \|\text{dev sym}(p_1 - p_2)(t)\|^2 dV = 0, \\
& \int_{\Omega} \|\text{Curl}(p_1 - p_2)(t)\|^2 dV = 0. \tag{5.5}
\end{aligned}$$

Since $p_1, p_2 \in \mathfrak{sl}(3)$ it follows that $\text{sym}(p_1 - p_2) = 0$ almost everywhere, i.e., $p_1 - p_2 \in \mathfrak{so}(3)$. Moreover, from the micro-hard boundary condition $\dot{p}_1 \cdot \tau = \dot{p}_2 \cdot \tau = 0$ we obtain

$p_1(x, t) \cdot \tau = p_2(x, t) \cdot \tau = p(x, 0) \cdot \tau$ which implies that $(p_1 - p_2) \cdot \tau = 0$ on Γ_D . But then $p_1 - p_2 = 0$ on Γ_D due to the skew-symmetry of the difference. However Curl controls all first partial derivatives on skew-symmetric matrices [45], therefore $p_1 - p_2 = 0$. Thus from Korn's first inequality we obtain uniqueness also for u . As a result: apart for the pure insulation condition all mentioned boundary conditions in (5.1) (and (5.2) ensure uniqueness of classical solutions except for the pure micro-free condition, in which case the skew-symmetric part of the difference of two solutions remains undetermined up to a constant skew-symmetric matrix. \blacksquare

5.2 Reformulation of the problem

The meaning of the flow rule is, recalling the definition of the subdifferential (3.48),

$$\dot{p} \in \partial\mathcal{X}(\Sigma^{\text{lin}}) \Leftrightarrow \mathcal{X}(\tilde{\Sigma}) \geq \mathcal{X}(\Sigma^{\text{lin}}) + \langle \dot{p}, \tilde{\Sigma} - \Sigma^{\text{lin}} \rangle \quad \forall \tilde{\Sigma} \in \mathcal{E}. \quad (5.6)$$

The Legendre transformation of \mathcal{X} is given, as is well known, by

$$R(\xi) = \mathcal{X}^*(\xi) = \begin{cases} \sigma_y \|\xi\| & \xi \in \mathfrak{sl}(3) \\ \infty & \xi \notin \mathfrak{sl}(3), \end{cases} \quad (5.7)$$

where R is also called the **dissipation potential** (notation: j in [19]). Here, for rate-independent processes, R is convex and homogeneous of grade one. It holds that

$$\begin{aligned} \text{sign}(\xi) &= \partial R(\xi) \\ &= \partial\mathcal{X}^*(\xi) = [\partial\mathcal{X}]^{-1}(\xi) = \begin{cases} \sigma_y \frac{\xi}{\|\xi\|} & \xi \neq 0, \xi \in \mathfrak{sl}(3) \\ \{\zeta \mid \|\text{dev } \zeta\| \leq \sigma_y\} & \xi = 0 \\ \emptyset & \xi \notin \mathfrak{sl}(3), \end{cases} \end{aligned} \quad (5.8)$$

and for a "gauge" $g : X \mapsto \overline{\mathbb{R}}, g(x) \geq 0, g(0) = 0$ with g convex and homogeneous of degree one it holds [19, p.77]: $\xi \in \partial g(x) \Leftrightarrow x \in \partial g^*(\xi)$. Hence, the **flow rule can be formulated equivalently** by writing (note that Σ^{lin} is not necessarily deviatoric)

$$\begin{aligned} \dot{p} \in \partial\mathcal{X}(\Sigma^{\text{lin}}) &\Leftrightarrow \Sigma^{\text{lin}} \in [\partial\mathcal{X}]^{-1}(\dot{p}) \Leftrightarrow \Sigma^{\text{lin}} \in \partial R(\dot{p}) \Leftrightarrow \\ R(\tilde{q}) &\geq R(\dot{p}) + \langle \Sigma^{\text{lin}}, \tilde{q} - \dot{p} \rangle \quad \forall \tilde{q} \in L^2([0, T], \mathfrak{sl}(3)). \end{aligned} \quad (5.9)$$

Integrating the former in space we note that

$$\int_{\Omega} R(\tilde{q}) \, dV \geq \int_{\Omega} R(\dot{p}) + \langle \Sigma^{\text{lin}}, \tilde{q} - \dot{p} \rangle \, dV \quad (5.10)$$

is good defined for all $\tilde{q} - \dot{p} \in L^2(0, T; L^1(\Omega, \mathfrak{sl}(3)))$ (p as a solution is already smoother), since we have that

$$\langle \Sigma^{\text{lin}}, \tilde{q} - \dot{p} \rangle = \langle \text{dev } \Sigma^{\text{lin}}, \tilde{q} - \dot{p} \rangle \leq \sigma_y \|\tilde{q} - \dot{p}\|, \quad (5.11)$$

from the flow rule. From (5.9)₂ it is easy to still recover the pointwise constraint on the deviatoric stresses. Since $\tilde{q}, \dot{p} \in \mathfrak{sl}(3)$ it holds

$$\langle \text{dev } \Sigma^{\text{lin}}, \tilde{q} - \dot{p} \rangle = \langle \Sigma^{\text{lin}}, \tilde{q} - \dot{p} \rangle \leq R(\tilde{q}) - R(\dot{p}) \leq \|R(\tilde{q}) - R(\dot{p})\| \leq \sigma_y \|\tilde{q} - \dot{p}\|. \quad (5.12)$$

Choosing $\tilde{q} \in \mathfrak{sl}(3)$ such that $\tilde{q} - \dot{p} = \text{dev } \Sigma^{\text{lin}}$ shows $\|\text{dev } \Sigma^{\text{lin}}\| \leq \sigma_y$. We have included this reverse calculation because this pointwise stress bound will be lost in our following weak reformulation due to the Curl-terms. This shows that the relation between the strong and weak formulation deserves detailed attention.

5.3 Strengthening of the boundary conditions for the plastic distortion

In order for us to be able to show existence and uniqueness of a subsequent weak formulation we need to strengthen the boundary and initial conditions. More precisely, we assume $p(x, 0) \cdot \tau = 0$, $x \in \Gamma_D$ and, moreover, for all $t \in (0, T)$

$$\begin{aligned} \text{sym } p(x, t) \cdot \tau &= 0, & x \in \Gamma_D, \\ \text{skew } p(x, t) \cdot \tau &= 0, & x \in \Gamma_D \Rightarrow \text{skew } p(x, t) = 0, \\ [\text{Curl sym } p(x, t)] \cdot \tau &= 0 \quad [\text{Curl skew } p(x, t)] \cdot \tau = 0, & x \in \partial\Omega. \end{aligned} \quad (5.13)$$

Remark 5.1 (Boundary conditions on the plastic distortion)

The boundary conditions imposed by the insulation condition in the geometrically exact case are not necessarily the same as those imposed by the need to show uniqueness in the geometrically linear setting. We could as well dispose of the condition $F_p(x, t) \cdot \tau = F_p(x, 0) \cdot \tau$ for $x \in \Gamma_D$ and assume then $\text{Curl } F_p \cdot \tau = 0$ on $\partial\Omega$. In this case, linearized uniqueness will be lost.

As an example consider the case of elastic energy minimization for $Q \in \text{SO}(3)$ with energy $\int_{\Omega} \|\text{D}_x Q\|^2 + \|\text{D}_x Q\|^4 \, dV$ together with natural boundary conditions. Since $\|Q\|^4 = 9$ for exact rotations we obtain boundedness of minimizing sequences $Q_k \in W^{1,4}(\Omega, \text{SO}(3))$ and establish the existence of a minimizer $Q \in C(\bar{\Omega}, \text{SO}(3))$, without Dirichlet boundary conditions on Q ! Now consider the geometrical linearization $Q = \mathbb{1} + A + \dots$, $A \in \mathfrak{so}(3)$. The linearized energy contribution reads $\int_{\Omega} \|\text{D}_x A\|^2 \, dV$. Consider minimizing sequences A_k . But $A_k \in \mathfrak{so}(3)$ can still be unbounded-only if we prescribe Dirichlet boundary conditions somewhere on $\partial\Omega$ can we conclude the boundedness of minimizing sequences and the existence of minimizers. We observe that the linearized model does need Dirichlet-boundary conditions in order to obtain existence where the nonlinear model does not.

5.4 The weak formulation of the problem

Let us re-formulate problem (4.12) with (5.10) in a weak sense. We set $V = H_0^1(\Omega, \Gamma_D, \mathbb{R}^3)$, the space of displacements with incorporated Dirichlet boundary conditions at $\Gamma_D \subset \partial\Omega$. Assume that solutions (u, p) to (4.12) exist with the regularity assumed in (4.11) so that all terms in (4.12) concerning the plastic variable p have a meaning in the strong sense, notably $\text{Curl } p \cdot \tau$ can be defined.

Multiply the first equation in (4.12) with test functions $(v - \dot{u}) \in L^2([0, T], H_0^1(\Omega, \Gamma_D, \mathbb{R}^3))$, integrate in space and use the boundary condition $(v - \dot{u})|_{\Gamma_D} = 0$ and the traction free condition on $\partial\Omega \setminus \Gamma_D$ in the sense of traces to obtain

$$\begin{aligned} 0 &= \int_{\Omega} \langle \sigma(x, t), \nabla v - \nabla \dot{u} \rangle - \langle f(x, t), v - \dot{u} \rangle \, dV \quad \forall v - \dot{u} \in L^2([0, T], V), \\ \sigma &= 2\mu \operatorname{sym}(\nabla u - p) + \lambda \operatorname{tr}[\nabla u - p] \mathbb{1}. \end{aligned} \quad (5.14)$$

Take (5.10) with

$$\tilde{q} = q \in \mathfrak{H} := H^1([0, T]; C^\infty(\bar{\Omega}; \mathfrak{sl}(3), p|_{\Gamma_D} \cdot \tau = 0)), \quad (5.15)$$

to obtain

$$0 \leq \int_{\Omega} R(q) - R(\dot{p}) - \langle \Sigma^{\operatorname{lin}}, q - \dot{p} \rangle \, dV \quad \forall q \in \mathfrak{H}, \quad (5.16)$$

insert the constitutive relation (4.12)₂ for $\Sigma^{\operatorname{lin}}$ and perform the (possible) partial integration on the Curl Curl-term using the boundary conditions of (4.12) for p , i.e., $\operatorname{Curl} p \cdot \tau = 0$ on $\partial\Omega \setminus \Gamma_D$ and $p \cdot \tau = 0$ on Γ_D (for this step the satisfaction of the insulation condition suffices) to get²⁰

$$\begin{aligned} 0 &\leq \int_{\Omega} R(q) - R(\dot{p}) - \langle \sigma - 2\mu h^+ \operatorname{dev} \operatorname{sym} p, q - \dot{p} \rangle, \\ &\quad + \mu L_c^2 \langle \operatorname{Curl} p, \operatorname{Curl}[q - \dot{p}] \rangle \, dV \quad \forall q \in \mathfrak{H}. \end{aligned} \quad (5.17)$$

Adding (5.14) and (5.17) we obtain the variational inequality: for almost all $t \in (0, T)$

$$\begin{aligned} \int_{\Omega} \langle f(x, t), v - \dot{u} \rangle \, dV &\leq \int_{\Omega} \langle \sigma(x, t), \nabla v - \nabla \dot{u} \rangle \, dV \\ &\quad + \int_{\Omega} R(q) - R(\dot{p}) - \langle \sigma - 2\mu h^+ \operatorname{dev} \operatorname{sym} p, q - \dot{p} \rangle \\ &\quad + \mu L_c^2 \langle \operatorname{Curl} p, \operatorname{Curl}[q - \dot{p}] \rangle \, dV \quad \forall (v, q) \in H^1([0, T]; V) \times \mathfrak{H}. \end{aligned} \quad (5.18)$$

On the space $Z := H^1([0, T]; V) \times \mathfrak{H}$ we may define a bilinear form $a : Z \times Z \mapsto \mathbb{R}$ for $w = (u_1, p_1)$, $z = (u_2, p_2)$

$$\begin{aligned} a(w, z) &= \int_{\Omega} 2\mu \langle \operatorname{sym}(\nabla u_1 - p_1), \operatorname{sym}(\nabla u_2 - p_2) \rangle + \lambda \operatorname{tr}[\nabla u_1 - p_1] \operatorname{tr}[\nabla u_2 - p_2] \\ &\quad + 2\mu h^+ \langle \operatorname{dev} \operatorname{sym} p_1, \operatorname{dev} \operatorname{sym} p_2 \rangle + \mu L_c^2 \langle \operatorname{Curl} p_1, \operatorname{Curl} p_2 \rangle \, dV \\ &= \int_{\Omega} 2\mu \langle \operatorname{sym}(\nabla u_1 - p_1), \operatorname{sym} \nabla u_2 \rangle + \lambda \operatorname{tr}[\nabla u_1 - p_1] \operatorname{tr}[\nabla u_2] - \langle \sigma, p_2 \rangle \\ &\quad + 2\mu h^+ \langle \operatorname{dev} \operatorname{sym} p_1, \operatorname{dev} \operatorname{sym} p_2 \rangle + \mu L_c^2 \langle \operatorname{Curl} p_1, \operatorname{Curl} p_2 \rangle \, dV. \end{aligned} \quad (5.19)$$

Let us also abbreviate $j(p) := \int_{\Omega} R(p) \, dV = \int_{\Omega} \mathcal{X}^*(p) \, dV$. Thus any strong solution (u, p) of (4.12) having the regularity (4.11) will satisfy the **preliminary weak primal problem of our gradient-plasticity formulation**, defined now.

²⁰It seems to be impossible to infer from (5.17) a pointwise bound on $\operatorname{dev} \Sigma^{\operatorname{lin}}$, see Lemma 5.6. This is the prize to be paid to work with the weak formulation.

Definition 5.2 (weak primal problem of gradient plasticity I)

We call

$$w(t) = (u(t), p(t)) \in H^1([0, T]; H_0^1(\Omega, \Gamma_D, \mathbb{R}^3)) \quad (5.20) \\ \times H^1([0, T]; \{\text{sym } p \in L^2(\Omega, \mathfrak{sl}(3)), \text{Curl } p \in L^2(\Omega), p|_{\Gamma_D} \cdot \tau = 0\}),$$

weak solution of the infinitesimal gradient plasticity model (4.12), if for almost all $t \in (0, T)$ it holds

$$\int_{\Omega} \langle f(x, t), v - \dot{u} \rangle dV \leq a \left(\begin{pmatrix} u \\ p \end{pmatrix}, \begin{pmatrix} v - \dot{u} \\ q - \dot{p} \end{pmatrix} \right) + j(q) - j(\dot{p}) \quad \forall (v, q) \in Z. \quad \blacksquare$$

The approach towards defining weak solutions taken in Definition 5.2 seems to be natural at first sight. However, while the set $\{C^\infty(\bar{\Omega}; \mathfrak{sl}(3), p|_{\Gamma_D} \cdot \tau = 0\}$ can be closed to a Hilbert-space under the norm $\|p\|_{\text{curl, sym}}^2 := \|\text{sym } p\|_{L^2(\Omega)}^2 + \|\text{Curl } p\|_{L^2(\Omega)}^2$, the ensuing Hilbert space might not be continuously embedded in $L^2(\Omega)$ and the continuous definition of traces giving $p|_{\Gamma_D} \cdot \tau = 0$ a precise meaning seems impossible.²¹

Therefore we propose to modify the weak formulation by incorporating the **stronger boundary conditions** in the formal derivation of the weak problem. Going back to inequality (5.18) we analyze the dislocations-density dependent term in more detail, invoking now the **stronger boundary conditions** (5.13) for p . Abbreviate momentarily $\zeta = q - \dot{p}$, let the smooth testfunction q satisfy $\text{sym } q \cdot \tau = \text{skew } q \cdot \tau = 0$ on Γ_D and consider

$$\int_{\Omega} \langle \text{Curl } p, \text{Curl } \zeta \rangle dV = \int_{\Omega} \langle \text{Curl}[\text{sym } p + \text{skew } p], \text{Curl}[\text{sym } \zeta + \text{skew } \zeta] \rangle dV \quad (5.21) \\ = \int_{\Omega} \langle \text{Curl } \text{sym } p, \text{Curl } \text{sym } \zeta \rangle + \langle \text{Curl } \text{skew } p, \text{Curl } \text{skew } \zeta \rangle \\ + \langle \text{Curl } \text{sym } p, \text{Curl } \text{skew } \zeta \rangle + \langle \text{Curl } \text{skew } p, \text{Curl } \text{sym } \zeta \rangle dV.$$

Since p satisfies the boundary conditions (5.13) and ζ satisfies $\text{sym } \zeta \cdot \tau = \text{skew } \zeta \cdot \tau = 0$ on Γ_D it follows that the two mixed sym / skew-terms vanish separately, cf. (5.40). Thus we may define accordingly a modified bilinear form $a_{\sharp} : Z \times Z \mapsto \mathbb{R}$ for $w = (u_1, p_1)$, $z = (u_2, p_2)$

$$a_{\sharp}(w, z) = \int_{\Omega} 2\mu \langle \text{sym}(\nabla u_1 - p_1), \text{sym}(\nabla u_2 - p_2) \rangle + \lambda \text{tr} [\nabla u_1 - p_1] \text{tr} [\nabla u_2 - p_2] \\ + 2\mu h^+ \langle \text{dev } \text{sym } p_1, \text{dev } \text{sym } p_2 \rangle \quad (5.22) \\ + \mu L_c^2 (\langle \text{Curl } \text{sym } p_1, \text{Curl } \text{sym } p_2 \rangle + \langle \text{Curl } \text{skew } p_1, \text{Curl } \text{skew } p_2 \rangle) dV.$$

Any strong solution (u, p) of (4.12) having the regularity (4.11) and satisfying in addition the stronger boundary conditions (5.13) will satisfy the **modified weak primal problem of our gradient-plasticity formulation**:

²¹Since p is not symmetric, this is not the space H_{curl} which would allow to specify tangential traces for p .

Definition 5.3 (weak primal problem of gradient plasticity II)

We call

$$\begin{aligned} w(t) = (u(t), p(t)) &\in H^1([0, T]; H_0^1(\Omega, \Gamma_D, \mathbb{R}^3)) \times H^1([0, T]; \mathcal{H}_\sharp), \\ \text{sym } p \cdot \tau = \text{skew } p \cdot \tau &= 0 \quad \text{on } \Gamma_D, \end{aligned} \quad (5.23)$$

weak solution of the infinitesimal gradient plasticity model (4.12), if for almost all $t \in (0, T)$ it holds

$$\int_{\Omega} \langle f(x, t), v - \dot{u} \rangle \, dV \leq a_{\sharp} \left(\begin{pmatrix} u \\ p \end{pmatrix}, \begin{pmatrix} v - \dot{u} \\ q - \dot{p} \end{pmatrix} \right) + j(q) - j(\dot{p}) \quad \forall (v, q) \in Z,$$

where the Hilbert-space \mathcal{H}_\sharp is defined in section (5.5). ■

Let us now see in what respect solutions in the sense of Definition 5.2 (for simplicity only) are related to the original strong formulation and what other type of relations they satisfy.

Corollary 5.4

Assume that a smooth solution (u, p) in the sense of Definition 5.2 satisfies additionally the **insulation condition**

$$\int_{\Omega} \sum_{i=1}^3 \text{Div} \left(\frac{d}{dt} p^i \times (\text{curl } p)^i \right) \, dV = \int_{\partial\Omega} \sum_{i=1}^3 \left\langle \frac{d}{dt} p^i \times (\text{curl } p)^i, \vec{n} \right\rangle \, dS \equiv 0. \quad (5.24)$$

Then (u, p) is a strong solution of (4.12) in the interior of the domain. If the boundary conditions of (4.12) are satisfied then this solution is a strong solution up to the boundary.

Proof. Obvious. ■

Corollary 5.5

Assume that (u, p) satisfy Definition 5.2. Then the weak form of balance of forces and the global energy inequality are satisfied.

Proof. Assume that $w = (u, p)$ is a solution of Definition 5.2. Test the variational inequality Definition 5.2 with both $(v, q) = (\xi + \dot{u}, p)$ and $(v, q) = (-\xi + \dot{u}, p)$. This shows

$$\int_{\Omega} \langle f(x, t), \xi \rangle \, dV \leq a(w, (\xi, 0)), \quad \int_{\Omega} \langle f(x, t), -\xi \rangle \, dV \leq a(w, (-\xi, 0)). \quad (5.25)$$

Hence from bilinearity, for all $\xi \in H^1([0, T]; V)$

$$\begin{aligned} \int_{\Omega} \langle f(x, t), \xi \rangle \, dV &= a(w, (\xi, 0)) \\ &= \int_{\Omega} 2\mu \langle \text{sym}(\nabla u - p), \text{sym}(\nabla \xi) \rangle + \lambda \text{tr} [\nabla u - p] \text{tr} [\nabla \xi] \, dV = \int_{\Omega} \langle \sigma, \nabla \xi \rangle \, dV, \end{aligned} \quad (5.26)$$

i.e., the weak form of balance of forces.

Assume again that $w = (u, p)$ is a solution of Definition 5.2 and test the variational inequality Definition 5.2 with both $(v, q) = (\xi + \dot{u}, \dot{p})$ and $(v, q) = (\xi + \dot{u}, -\dot{p})$. This shows

$$\begin{aligned} \int_{\Omega} \langle f(x, t), \xi \rangle dV &\leq a(w, (\xi, 0)), \quad \text{no new information} \\ \int_{\Omega} \langle f(x, t), \xi \rangle dV &\leq a(w, (\xi, -2\dot{p})). \end{aligned} \quad (5.27)$$

Hence we obtain

$$\begin{aligned} \int_{\Omega} \langle f(x, t), \xi \rangle dV &\leq a(w, (\xi, \dot{p})) \\ &= \int_{\Omega} 2\mu \langle \text{sym}(\nabla u - p), \text{sym} \nabla \xi \rangle + \lambda \text{tr} [\nabla u - p] \text{tr} [\nabla \xi] - \langle \sigma, \dot{p} \rangle \\ &\quad + 2\mu h^+ \langle \text{dev sym } p, \text{dev sym } \dot{p} \rangle + \mu L_c^2 \langle \text{Curl } p, \text{Curl } \dot{p} \rangle dV \end{aligned} \quad (5.28)$$

and further

$$\begin{aligned} \int_{\Omega} \langle f(x, t), \xi \rangle dV &\leq a(w, (\xi, -2\dot{p})) \\ &= \int_{\Omega} 2\mu \langle \text{sym}(\nabla u - p), \text{sym} \nabla \xi \rangle + \lambda \text{tr} [\nabla u - p] \text{tr} [\nabla \xi] + 2\langle \sigma, \dot{p} \rangle \\ &\quad - 4\mu h^+ \langle \text{dev sym } p, \text{dev sym } \dot{p} \rangle - 2\mu L_c^2 \langle \text{Curl } p, \text{Curl } \dot{p} \rangle dV \end{aligned} \quad (5.29)$$

which shows, using balance of forces

$$\begin{aligned} 0 &\leq \int_{\Omega} \langle \sigma, \dot{p} \rangle - 2\mu h^+ \langle \text{dev sym } p, \text{dev sym } \dot{p} \rangle - \mu L_c^2 \langle \text{Curl } p, \text{Curl } \dot{p} \rangle dV \\ 0 &\geq \int_{\Omega} \langle \sigma, -\dot{p} \rangle + 2\mu h^+ \langle \text{dev sym } p, \text{dev sym } \dot{p} \rangle + \mu L_c^2 \langle \text{Curl } p, \text{Curl } \dot{p} \rangle dV \Rightarrow \\ 0 &\geq \int_{\Omega} \frac{d}{dt} W(\nabla u(x, t_0), p(t), \text{Curl } p(t)) dV. \end{aligned} \quad (5.30)$$

Thus we get the global a priori energy inequality back although we might not be able to speak about boundary values for $\text{Curl } p \cdot \tau = 0$. \blacksquare

The next statement is included in order to understand better the difference between smooth weak and strong solutions of Definition 5.2.

Lemma 5.6

Assume that (u, p) is a smooth weak solution in the sense of Definition 5.2. Then for all $q \in C^\infty(\Omega, \mathfrak{sl}(3))$, $q|_{\Gamma_D} \cdot \tau = 0$ it holds

$$\begin{aligned} \int_{\Omega} R(2\dot{p}) - R(q) dV &\leq \int_{\Omega} \langle \sigma - 2\mu h^+ \text{dev sym } p, q - \dot{p} \rangle + \mu L_c^2 \langle \text{Curl } \text{Curl } p, q - \dot{p} \rangle dV \\ &\quad + \int_{\partial\Omega \setminus \Gamma_D} \langle \text{Curl } p \times (q - \dot{p}), N \rangle dS \leq \int_{\Omega} R(2\dot{p} - q) dV. \end{aligned} \quad (5.31)$$

Proof. Since balance of forces is satisfied for a solution (u, p) of Definition 5.2 we have from (5.18) that

$$0 \leq \int_{\Omega} R(q) - R(\dot{p}) - \langle \sigma - 2\mu h^+ \operatorname{dev} \operatorname{sym} p, q - \dot{p} \rangle + \mu L_c^2 \langle \operatorname{Curl} p, \operatorname{Curl}[q - \dot{p}] \rangle \, dV \quad (5.32)$$

for all $q \in C^\infty(\Omega, \mathfrak{sl}(3))$. Since p is smooth and $p \cdot \tau = q \cdot \tau = 0$ on Γ_D we may integrate partially to obtain

$$\begin{aligned} 0 \leq & \int_{\Omega} R(q) - R(\dot{p}) - \langle \sigma - 2\mu h^+ \operatorname{dev} \operatorname{sym} p, q - \dot{p} \rangle + \mu L_c^2 \langle \operatorname{Curl} \operatorname{Curl} p, q - \dot{p} \rangle \, dV \\ & + \int_{\partial\Omega \setminus \Gamma_D} \langle \operatorname{Curl} p \times (q - \dot{p}), N \rangle \, dS. \end{aligned} \quad (5.33)$$

Now we test with $q = q_1$ and $q = q_2 = 2\dot{p} - q_1$ such that $q_1 - \dot{p} = -(q_2 - \dot{p})$. Thus we obtain

$$\begin{aligned} \int_{\Omega} R(\dot{p}) - R(q_1) \, dV \leq & \int_{\Omega} \langle \sigma - 2\mu h^+ \operatorname{dev} \operatorname{sym} p, q - \dot{p} \rangle + \mu L_c^2 \langle \operatorname{Curl} \operatorname{Curl} p, q - \dot{p} \rangle \, dV \\ & + \int_{\partial\Omega \setminus \Gamma_D} \langle \operatorname{Curl} p \times (q - \dot{p}), N \rangle \, dS \leq \int_{\Omega} R(2\dot{p} - q_1) - R(\dot{p}) \, dV. \end{aligned}$$

Rearranging and using the one-homogeneity of R yields

$$\begin{aligned} \int_{\Omega} R(2\dot{p}) - R(q_1) \, dV \leq & \int_{\Omega} \langle \sigma - 2\mu h^+ \operatorname{dev} \operatorname{sym} p, q - \dot{p} \rangle + \mu L_c^2 \langle \operatorname{Curl} \operatorname{Curl} p, q - \dot{p} \rangle \, dV \\ & + \int_{\partial\Omega \setminus \Gamma_D} \langle \operatorname{Curl} p \times (q - \dot{p}), N \rangle \, dS \leq \int_{\Omega} R(2\dot{p} - q_1) \, dV. \quad \blacksquare \end{aligned}$$

Remark 5.7

It is not obvious how to strengthen the statement in Lemma 5.6 by judiciously choosing the boundary values of the test-functions in order to conclude that a smooth weak solution p will assume the boundary conditions $\operatorname{Curl} p \cdot \tau = 0$ on $\partial\Omega \setminus \Gamma_D$ required for a strong solution. This is usually done (following the method connecting smooth weak and strong solutions of the Neumann-problem for the Laplace-operator) by showing that the second derivatives in the bulk must vanish which allows one to conclude that the boundary term must also vanish and that, necessarily, the smooth weak solution satisfies the Neumann condition strongly. The same recipe would work here, provided that the R -related dissipation terms were absent.

Remark 5.8

Altogether, the weak solution satisfies the a priori energy inequality which was one of the motivations for the insulation condition. At this moment, no statement can be made, whether the insulation condition does hold for the weak solution found (if we pose $\dot{p} = 0$ on $\partial\Omega$ then it does hold trivially, and this condition is possible to formulate within the weak framework).

If Definition 5.2 admits a unique solution then it satisfies automatically the global energy inequality. For such a solution it is, however, not possible to speak of boundary

conditions giving $\text{Curl } p \cdot \tau = 0$ any meaning. In this respect we may speculate that the solution of Definition 5.2 is an "interior approximation" of the original problem. This gap between solutions of Definition 5.2 and solutions of the original problem (4.12) usually does not occur in classical plasticity with linear kinematical hardening but without gradient dependence. Thus we see that the gradient-plasticity model differentiates profoundly between the local and the nonlocal different formulations.

Open problem: does a smooth solution in the sense of Definition 5.2 necessarily satisfy the insulation condition?

5.5 Existence of weak solutions

In the following we denote the linear functional of applied loads by ℓ and abbreviate $\ell(w) = \int_{\Omega} \langle f(x, t), w \rangle \, dV$. In order to prove the existence of weak solutions in the sharpened sense of Definition 5.3, we use the following abstract result for variational inequalities.

Theorem 5.9 (Existence and uniqueness for variational inequality)

Let $H(\Omega)$ be a Hilbert space and let W be a closed convex subset of the Hilbert space $Z = H^1([0, T]; H(\Omega))$ and consider the problem of finding $w \in W$ such that

$$\forall z \in W : \quad a(w, z - \dot{w}) + j(z) - j(\dot{w}) - \ell(z - \dot{w}) \geq 0. \quad (5.34)$$

Assume that the following hold:

1. the bilinear form $a(\cdot, \cdot)$ is symmetric, continuous on Z , and coercive on W , i.e.,

$$\begin{aligned} a(w, z) &\leq C^+ \|w\|_W \|z\|_W \quad \forall w, z \in Z, \\ a(z, z) &\geq C^+ \|z\|_W^2 \quad \forall z \in W. \end{aligned} \quad (5.35)$$

2. the linear form of external loads ℓ is bounded, i.e., $\|\ell(z)\| \leq C^+ \|z\|_W$.
3. the functional j is non-negative, convex, positively homogeneous of grade one and Lipschitz-continuous, i.e.,

$$\forall s \in \mathbb{R} : \quad j(sw) = |s| j(w), \quad |j(z) - j(w)| \leq L \|z - w\|_W. \quad (5.36)$$

Then the problem (5.34) has a unique solution $w(t) \in W$.

Proof. The proof is given in Theorem 7.3 in [19, p.166] by a time-discretization of the variational inequality and passage to the limit using the coercivity of the bilinear form and the very special properties of j . It is complementing ideas given in [35]. ■

Remark 5.10

The method of proof cannot easily be extended to evolution problems with non-associative \mathfrak{f} instead of associative $\partial\mathcal{X}$. Mielkes inventive new energetic formulation [33] of the rate-independent finite-strain case can be seen as a generalization of this method.

To show that the bilinear form a_{\sharp} satisfies the assumptions of this theorem, we need to introduce a new Hilbert-space \mathcal{H}_{\sharp} , which we define and investigate first. To this end define the sets

$$\begin{aligned}\mathcal{X}_{\sharp}^0 &:= \{p \in C^\infty(\overline{\Omega}, \mathbb{M}^{3 \times 3}) \mid \text{skew } p(x) \cdot \tau = 0, x \in \Gamma_D, \text{ Curl sym } p \cdot \tau = 0, x \in \partial\Omega \setminus \Gamma_D\}, \\ \mathcal{X}_{\sharp} &:= \{p \in C^\infty(\overline{\Omega}, \mathbb{M}^{3 \times 3}) \mid \text{skew } p(x) \cdot \tau = 0, x \in \Gamma_D\},\end{aligned}\quad (5.37)$$

where $\partial\Omega$ is assumed to have C^1 -boundary. Clearly $\mathcal{X}_{\sharp}^0 \subset \mathcal{X}_{\sharp}$. On \mathcal{X}_{\sharp}^0 we have the orthogonality relation (this boundary condition suffices! and partial integration)

$$\|\text{Curl } p\|_{L^2(\Omega)}^2 = \|\text{Curl sym } p\|_{L^2(\Omega)}^2 + \|\text{Curl skew } p\|_{L^2(\Omega)}^2. \quad (5.38)$$

To see this we compute for $\zeta \in \mathcal{X}_{\sharp}^0$

$$\begin{aligned}\|\text{Curl}(\text{sym } \zeta + \text{skew } \zeta)\|^2 &= \|\text{Curl sym } \zeta\|^2 + 2\langle \text{Curl sym } \zeta, \text{Curl skew } \zeta \rangle \\ &\quad + \|\text{Curl skew } \zeta\|^2.\end{aligned}\quad (5.39)$$

For the middle term we obtain

$$\begin{aligned}\int_{\Omega} \langle \text{Curl sym } \zeta, \text{Curl skew } \zeta \rangle \, dV &= \int_{\Omega} \langle \text{Curl Curl sym } \zeta, \text{skew } \zeta \rangle \, dV \\ + \int_{\partial\Omega \setminus \Gamma_D} \langle \text{Curl sym } \zeta \times \text{skew } \zeta, \vec{N} \rangle \, dS &+ \int_{\Gamma_D} \langle \text{Curl sym } \zeta \times \text{skew } \zeta, \vec{N} \rangle \, dS \\ &= \int_{\Omega} \underbrace{\langle \text{Curl Curl sym } \zeta, \text{skew } \zeta \rangle}_{\in \text{Sym}(3) \text{ [14, p.12]}} \, dV = 0.\end{aligned}\quad (5.40)$$

Thus we may define a quadratic form

$$\begin{aligned}\|p\|_{\sharp}^2 &:= \|\text{sym } p\|_{L^2(\Omega)}^2 + \|\text{Curl sym } p\|_{L^2(\Omega)}^2 + \|\text{Curl skew } p\|_{L^2(\Omega)}^2 \\ &= \|\text{sym } p\|_{L^2(\Omega)}^2 + \|\text{Curl } p\|_{L^2(\Omega)}^2 = \|p\|_{\text{curl, sym}}^2 \quad \text{on } \mathcal{X}_{\sharp}^0.\end{aligned}\quad (5.41)$$

Let us show that this defines a norm on \mathcal{X}_{\sharp} .

Lemma 5.11

$\|p\|_{\sharp}$ is a norm on \mathcal{X}_{\sharp} .

Proof. Positivity, homogeneity and the triangle inequality are clear. We need only to show that

$$p \in \mathcal{X}_{\sharp}, \quad \|p\|_{\sharp} = 0 \Rightarrow p \equiv 0. \quad (5.42)$$

Since p is smooth we have

$$\begin{aligned}\|p\|_{\sharp} = 0 &\Rightarrow \|\text{sym } p\|_{L^2(\Omega)} = 0, \text{ and } \|\text{Curl } p\|_{L^2(\Omega)} = 0, \\ &\Rightarrow \text{sym } p(x) = 0 \Rightarrow p(x) = A(x) \in \mathfrak{so}(3), \text{ Curl } p(x) = \text{Curl } A(x) = 0.\end{aligned}\quad (5.43)$$

However, Curl is isomorphic to ∇ on $C^\infty(\Omega, \mathfrak{so}(3))$ [45], thus the former implies that $A(x) = \text{const.}$. Moreover

$$[\text{skew } p(x)].\tau_1(x) = [\text{skew } p(x)].\tau_2(x) = 0 \Rightarrow A.\tau_1 = A.\tau_2 = 0 \Rightarrow \text{rank}(A) \leq 1. \quad (5.44)$$

Since a skew-symmetric matrix A in \mathbb{R}^3 has either rank two or rank zero (in which case it is zero) we conclude that $A \equiv 0$. Thus $p = A = 0$. \blacksquare

Corollary 5.12

$\|p\|_{\text{curl, sym}}$ is also a norm on \mathcal{X}_\sharp . \blacksquare

Finally, we take the completion of the encompassing space \mathcal{X}_\sharp with respect to the norm $\|\cdot\|_\sharp$ and define

$$\mathcal{H}_\sharp := \overline{\mathcal{X}_\sharp}^{\|\cdot\|_\sharp}, \quad (5.45)$$

making \mathcal{H}_\sharp into a Hilbert-space. Thus we have shown that $\mathcal{H}_\sharp(\Omega, \mathbb{M}^{3 \times 3})$ is a Hilbert-space with scalar product

$$\begin{aligned} \langle p_1, p_2 \rangle_\sharp &= \int_\Omega \langle \text{sym } p_1, \text{sym } p_2 \rangle + \langle \text{Curl sym } p_1, \text{Curl sym } p_2 \rangle \\ &\quad + \langle \text{Curl skew } p_1, \text{Curl skew } p_2 \rangle \, dV. \end{aligned} \quad (5.46)$$

The space \mathcal{H}_\sharp is continuously embedded in $L^2(\Omega, \mathbb{M}^{3 \times 3})$.

Lemma 5.13 (Continuous embedding of \mathcal{H}_\sharp in $L^2(\Omega)$)

The space \mathcal{H}_\sharp is continuously embedded in $L^2(\Omega, \mathbb{M}^{3 \times 3})$, i.e.,

$$\exists C^+ : \forall \zeta \in \mathcal{H}_\sharp \quad \|\zeta\|_{L^2(\Omega)} \leq C^+ \|\zeta\|_\sharp. \quad (5.47)$$

Proof. We show the inequality for functions in \mathcal{X}_\sharp and pass then to the limit by density. Decomposing $\zeta = \text{sym } \zeta + \text{skew } \zeta$ and using that (pointwise and integrated)

$$\|\zeta\|^2 = \|\text{sym } \zeta\|^2 + \|\text{skew } \zeta\|^2 \Rightarrow \|\zeta\|_{L^2(\Omega)}^2 \leq \|\zeta\|_\sharp^2 + \|\text{skew } \zeta\|_{L^2(\Omega)}^2, \quad (5.48)$$

it remains to bound $\|\text{skew } \zeta\|_{L^2(\Omega)}^2$ in terms of $\|\zeta\|_\sharp^2$. However,

$$\begin{aligned} \|\text{skew } \zeta\|_{L^2(\Omega)}^2 &\leq \|\text{skew } \zeta\|_{H^1(\Omega)}^2 \leq C^+ \|\nabla \text{skew } \zeta\|_{L^2(\Omega)} \\ &\leq C^+ \|\text{Curl skew } \zeta\|_{L^2(\Omega)}^2 \leq C^+ \|\zeta\|_\sharp^2, \end{aligned} \quad (5.49)$$

where we have used in the first line Poincaré's-inequality for functions $\zeta \in \mathcal{X}_\sharp$ that satisfy automatically $\text{skew } \zeta|_{\Gamma_D} = 0$ and in the second line that Curl bounds ∇ (pointwise) on $\mathfrak{so}(3)$. \blacksquare

Lemma 5.14

The linear space $H^1(\Omega, \mathbb{M}^{3 \times 3}) \cap \{\text{skew } p(x) = 0, x \in \Gamma_D\}$ (boundary term in the sense of traces) is contained in \mathcal{H}_\sharp .

Proof. Note first that $C^\infty(\Omega, \mathbb{M}^{3 \times 3}) \cap \{\text{skew } p(x) = 0, x \in \Gamma_D\} \subset X_\sharp$ and that

$$\forall p \in X_\sharp : \quad \|p\|_\sharp \leq C^+ \|p\|_{H^1(\Omega)}. \quad (5.50)$$

Choose $\phi \in H^1(\Omega, \mathbb{M}^{3 \times 3}) \cap \{\text{skew } p(x) = 0, x \in \Gamma_D\}$. Then there is a sequence $\phi_n \in C^\infty(\Omega, \mathbb{M}^{3 \times 3}) \cap \{\text{skew } p(x) = 0, x \in \Gamma_D\}$ such that $\phi_n \rightarrow \phi$ strongly in H^1 . Since

$$\|\phi - \phi_n\|_\sharp \leq \|\phi - \phi_n\|_{H^1(\Omega)}, \quad (5.51)$$

this implies $\|\phi - \phi_n\|_\sharp \rightarrow 0$. Hence ϕ is contained in the closure of \mathcal{X}_\sharp w.r.t. to the norm $\|\cdot\|_\sharp$. ■

Remark 5.15

The new space \mathcal{H}_\sharp is not compactly embedded in $L^2(\Omega, \mathbb{M}^{3 \times 3})$. To see this consider a sequence $p_k = \nabla u_k$, bounded in \mathcal{H}_\sharp . Because of the gradient structure $\text{Curl } p_k \equiv 0$ but $p_k = \nabla u_k$ need not converge.

Lemma 5.16 (\mathcal{H}_\sharp and boundary values)

The space \mathcal{H}_\sharp admits continuous traces in the sense that for tangential vectors τ the following terms can be defined on $\partial\Omega$

$$\text{sym } p(x, t) \cdot \tau \in L^2(\partial\Omega), \quad \text{skew } p(x, t) \cdot \tau \in L^2(\partial\Omega). \quad (5.52)$$

Proof. Since $\text{sym } p \in L^2(\Omega)$ and $\text{Curl } \text{sym } p \in L^2(\Omega)$ the tangential trace $\text{sym } p \cdot \tau$ can be defined. Similarly, for $\text{skew } p \in L^2(\Omega)$ and $\text{Curl } \text{skew } p \in L^2(\Omega)$ the tangential trace $\text{skew } p \cdot \tau$ can be defined. ■

Therefore, in this space, the boundary condition $p \cdot \tau = 0$ on Γ_D is well defined in the sense of traces. Moreover, we have the characterization

$$\mathcal{H}_\sharp = \{\text{sym } p \in H_{\text{curl}}(\Omega), \text{ skew } p \in H_0^1(\Omega, \Gamma_D, \mathfrak{so}(3))\}. \quad (5.53)$$

Having presented our Hilbert-space we are now ready to announce our final result.

Theorem 5.17 (Existence and uniqueness of weak solutions)

The mixed variational inequality (5.3) together with the strengthened boundary condition (5.13) has a unique weak solution in $Z = H^1(0, T; H(\Omega))$ with

$$H(\Omega) := H_0^1(\Omega, \Gamma_D, \mathbb{R}^3) \times \mathcal{H}_\sharp. \quad (5.54)$$

Proof. In order to apply the abstract framework Theorem 5.34, we define the closed, convex subset of the Hilbert-space \mathcal{H}_\sharp

$$K = \{p \in \mathcal{H}_\sharp, \quad \text{tr } [p] = 0, \quad \text{sym } p(x, t) \cdot \tau = 0, \quad \text{skew } p(x, t) \cdot \tau = 0, \quad x \in \Gamma_D\},$$

and define

$$H(\Omega) := H_0^1(\Omega, \Gamma_D, \mathbb{R}^3) \times \mathcal{H}_\sharp, \quad W := H_0^1(\Omega, \Gamma_D, \mathbb{R}^3) \times K, \quad Z := H^1([0, T]; H(\Omega)).$$

It is easy to see that the bilinear form a_{\sharp} , defined in (5.19) is symmetric and continuous on Z . Moreover, for $z = (u, p) \in W$ we have

$$\begin{aligned}
a_{\sharp}(z, z) &= \int_{\Omega} 2\mu \langle \text{sym}(\nabla u - p), \text{sym}(\nabla u - p) \rangle + \lambda \text{tr} [\nabla u - p] \text{tr} [\nabla u - p] \\
&\quad + 2\mu h^+ \langle \text{dev sym } p, \text{dev sym } p \rangle \\
&\quad + \mu L_c^2 (\langle \text{Curl sym } p, \text{Curl sym } p \rangle + \langle \text{Curl skew } p, \text{Curl skew } p \rangle) \, dV \\
&\geq \int_{\Omega} 2\mu \|\text{sym}(\nabla u - p)\|^2 + 2\mu h^+ \|\text{dev sym } p\|^2 \\
&\quad + \mu L_c^2 (\|\text{Curl sym } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&= \int_{\Omega} 2\mu (\|\text{sym } \nabla u\|^2 - 2\langle \text{sym } \nabla u, \text{sym } p \rangle + \|\text{sym } p\|^2) + 2\mu h^+ \|\text{dev sym } p\|^2 \\
&\quad + \mu L_c^2 (\|\text{Curl } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&\geq \int_{\Omega} 2\mu (\|\text{sym } \nabla u\|^2 - 2\|\text{sym } \nabla u\| \|\text{sym } p\| + \|\text{sym } p\|^2) + 2\mu h^+ \|\text{dev sym } p\|^2 \\
&\quad + \mu L_c^2 (\|\text{Curl sym } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&\quad \text{Cauchy-Schwarz and Young's inequality} \\
&\geq \int_{\Omega} 2\mu \left(\|\text{sym } \nabla u\|^2 - \varepsilon \|\text{sym } \nabla u\|^2 - \frac{1}{\varepsilon} \|\text{sym } p\|^2 + \|\text{sym } p\|^2 \right) + 2\mu h^+ \|\text{dev sym } p\|^2 \\
&\quad + \mu L_c^2 (\|\text{Curl sym } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&= \int_{\Omega} 2\mu (1 - \varepsilon) \|\text{sym } \nabla u\|^2 + 2\mu (1 + h^+ - \frac{1}{\varepsilon}) \|\text{dev sym } p\|^2 \\
&\quad + \mu L_c^2 (\|\text{Curl sym } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&\text{choose } \varepsilon = (1 + \frac{h^+}{2})^{-1} \\
&\geq \int_{\Omega} \mu h^+ \|\text{sym } \nabla u\|^2 + \mu h^+ \|\text{dev sym } p\|^2 \\
&\quad + \mu L_c^2 (\|\text{Curl sym } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&\quad \text{since } p \in \mathfrak{sl}(3) \text{ it follows} \\
&= \int_{\Omega} \mu h^+ \|\text{sym } \nabla u\|^2 + \mu h^+ \|\text{sym } p\|^2 + \mu L_c^2 (\|\text{Curl sym } p\|^2 + \|\text{Curl skew } p\|^2) \, dV \\
&\geq \mu \left(h^+ \|\text{sym } \nabla u\|_{L^2(\Omega)}^2 + \min(h^+, L_c^2) \|p\|_{\sharp}^2 \right) \\
&\quad \text{using Korn's inequality for the displacement } u \in H_0^1(\Omega, \Gamma_D, \mathbb{R}^3) \\
&\geq \mu \left(h^+ C_K \|u\|_{H^1(\Omega)}^2 + \min(h^+, L_c^2) \|p\|_{\sharp}^2 \right).
\end{aligned}$$

Thus a_{\sharp} is positive definite on W . Moreover, $j(q) = \int_{\Omega} R(q) \, dV$ is one homogeneous and Lipschitz, due to (5.7). We have shown that within these spaces the problem (5.3) admits a unique weak solution. \blacksquare

Remark 5.18

Since we needed stronger boundary conditions for the existence of weak solutions than were needed for uniqueness of strong solutions the relation between smooth weak solutions and strong solutions is not entirely clear: even if strong solutions exist for the weaker boundary condition the unique weak solution need not coincide with it.

6 Discussion

The classical elasto-perfectly plastic Prandtl-Reuss model with kinematic hardening has been extended to include a weak nonlocal interaction of the plastic distortion by introducing the dislocation density in the Helmholtz free energy. The evolution equation for plasticity follows by an application of the second law of thermodynamics in the efficient formulation proposed by Maugin [27] together with a sufficient condition guaranteeing the insulation condition. This is done in a finite-strain setting based on the multiplicative decomposition. We apply a strict principle of referential, intermediate and spatial covariance. Referential covariance severely restricts the choice of the hardening contribution. However, full covariance w.r.t. constant rotations does not reduce the gradient plasticity model to a dependence on the plastic metric $C_p = F_p^T F_p$, in contrast to the classical case without gradients. In this context the gradient plasticity model allows to differentiate in more detail between form-invariance under all rotations (covariance for local model) and form-invariance under constant rotations (covariance for non-local model). The question of the correct invariance requirements to be satisfied in the multiplicative decomposition has been raised many times in the literature. Our development shows that this question has a new answer in the non-local setting: for full covariance with respect to rigid rotations of the reference, intermediate and spatial configuration in the multiplicative decomposition the model should satisfy the condition (3.38).

A geometrically linear version of the model is also derived. The proposed gradient plasticity model approximates formally the classical model in the large scale limit $L_c = 0$. For the rate-independent infinitesimal strain model the following has been obtained: uniqueness of strong solutions with micro-free/hard boundary conditions and that a weak formulation can be recast into a mixed variational inequality whose well-posedness can be shown in a suitable Hilbert-space. In the future we would like to extend our analysis to cover more general flow rules: rate-dependent viscoplasticity and non-associative formulations. In this respect it seems possible to use similar ideas as in [2]. Moreover, one should show stability as $L_c \rightarrow 0$. From a physical point of view it would be tempting to couple isotropic local hardening (covering effects of statistically stored dislocations) with the nonlocal kinematical hardening (due to geometrically necessary dislocations) and to omit the local Prager kinematical hardening term altogether.

It is remarked that in the above framework it seems that the rate-independent models are simpler to treat with than the rate dependent models. A shortcoming of the analysis is its inability to show that a smooth weak solution satisfies the boundary conditions which have been used in the derivation of the weak problem. This is object of ongoing research.

It remains also to be seen whether this formulation of gradient plasticity is not only

weakly well-posed but also amenable to an efficient numerical implementation. The introduction of a plastic length scale $L_c > 0$, which acts as a localization limiter should be compared to the Cosserat elasto-plasticity model [41, 43, 40, 44, 42] which also has the ability to remove the mesh-sensitivity. For the Cosserat model it is already shown that this can be implemented in a “cheap” way. Currently, the dislocation based plasticity model is being implemented, however, directly in the finite strain setting [46].

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8 Notation

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with Lipschitz boundary $\partial\Omega$ and let Γ be a smooth subset of $\partial\Omega$ with non-vanishing 2-dimensional Hausdorff measure. We denote by $\mathbb{M}^{3 \times 3}$ the set of real 3×3 second order tensors, written with capital letters. The standard Euclidean scalar product on $\mathbb{M}^{3 \times 3}$ is given by $\langle X, Y \rangle_{\mathbb{M}^{3 \times 3}} = \text{tr}[XY^T]$, and thus the Frobenius tensor norm is $\|X\|^2 = \langle X, X \rangle_{\mathbb{M}^{3 \times 3}}$ (we use these symbols indifferently for tensors and vectors). The identity tensor on $\mathbb{M}^{3 \times 3}$ will be denoted by $\mathbb{1}$, so that $\text{tr}[X] = \langle X, \mathbb{1} \rangle$. We let Sym and PSym denote the symmetric and positive definite symmetric tensors respectively. We adopt the usual abbreviations of Lie-algebra theory, i.e. $\mathfrak{so}(3) := \{X \in \mathbb{M}^{3 \times 3} \mid X^T = -X\}$ are skew symmetric second order tensors and $\mathfrak{sl}(3) := \{X \in \mathbb{M}^{3 \times 3} \mid \text{tr}[X] = 0\}$ are traceless tensors. We set $\text{sym}(X) = \frac{1}{2}(X^T + X)$ and $\text{skew}(X) = \frac{1}{2}(X - X^T)$ such that $X = \text{sym}(X) + \text{skew}(X)$. For $X \in \mathbb{M}^{3 \times 3}$ we set for the deviatoric part $\text{dev} X = X - \frac{1}{3} \text{tr}[X] \mathbb{1} \in \mathfrak{sl}(3)$. For a second order tensor X we let $X.e_i$ be the application of the tensor X to the column vector e_i .