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# Remarks on Invariant Modelling in Finite Strain Gradient Plasticity

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*I discuss invariance conditions arising in 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 flow rule for $F_p$ is assumed which can be derived by an underlying thermodynamic potential involving as plastic gradient $\operatorname{Curl} F_p$. The proposed formulation is supposed to be form-invariant w.r.t. arbitrary 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 $C_p = F_p^T F_p$. This is contrary to the case of the local theory without gradients on the plastic transformation $F_p$ in which case the same form-invariance conditions reduce the model to a dependence on $C_p$ [3].*

## 1 Introduction

This article addresses a form-invariant description of a gradient plasticity model. There is an abundant literature on gradient plasticity formulations [20, 21], in most cases letting the yield-stress depend also on some higher derivative of a scalar measure of accumulated plastic distortion [4]. The finite strain model I 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 [9], the dislocation density into the underlying thermodynamic potential. The corresponding flow rule can then be extracted from an extended principle of maximal dissipation based on the development in Maugin [14], but we will not focus on the flow rule here. Models, similar in spirit to our formulation, may be found in [16, 10].

Instead of incorporating a $\operatorname{Curl} F_p$-term in the thermodynamical potential it has been suggested to add a $\operatorname{Curl} F_p$-related term directly to the time-incremental update-potential [19] in the description of subgrain dislocation structures. It seems therefore worthwhile to investigate the general structure of gradient plasticity models.

This contribution is organized as follows: first, I recall one possibility for a basic modelling of multiplicative gradient plasticity. Then I discuss spatial, intermediate and referential form-invariance under arbitrary constant rotations. This seems to be a new approach as far as gradient plasticity is concerned. As a result, our finite strain model (the underlying thermodynamic potential) is materially frame-indifferent and isotropic w.r.t. both the reference configuration and the intermediate configuration. Nevertheless, the model cannot be reduced to depend only on the plastic metric $C_p = F_p^T F_p$, because of the presence of plastic gradients. The relevant notation is found in the appendix.

## 2 The Gradient Plasticity Model at Finite Strain

### 2.1 The Multiplicative Decomposition

Consider the well-known multiplicative decomposition [7, 8] of the deformation gradient $F = \nabla\varphi$ into elastic and plastic parts

$$F = F_e \cdot F_p \,. \tag{1}$$

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 additionally assumes this split to be of the form

$$F_p : T_x\Omega_{\rm ref} \mapsto T_x\Omega_{\rm ref}\,, \quad F_e : T_x\Omega_{\rm ref} \mapsto T_{\varphi(x)}\Omega_{\rm act}\,, \quad F : T_x\Omega_{\rm ref} \mapsto T_{\varphi(x)}\Omega_{\rm act}\,, \tag{2}$$

where $\Omega_{\rm ref}$ and $\Omega_{\rm act}$ are the referential and actual configuration respectively. Moreover, $F_p$ is uniquely constitutively determined by a flow rule describing the slip kinematics on preferred glide planes [9].

At the continuum level, however, the multiplicative decomposition (1) is merely a nonlinear generalization of the classical additive decomposition of the small strain tensor into elastic and plastic parts. In this case a constitutive assumption like (2) is not mandatory and the question of the uniqueness of this decomposition has been raised several times in the literature, since, formally it is always possible to write

$$F = F_e\,F_p = F_e\,Q^T\,Q\,F_p = F_e^*\,F_p^*\,, \tag{3}$$

with $Q \in {\rm SO}(3)$ an arbitrary rigid rotation.[1] In this contribution, I consider the split (1) as void of any additional microstructural information regarding the nature of $F_p$, contrary to (2). Since I assume that I do not know how to choose the rigid rotation in (3) a specific choice of rotation should be without consequence. This is leading to an additional invariance requirement on the intermediate configuration: all possible selections of the intermediate configuration are treated as equal. It is clear that such a strong invariance requirement is subject to discussion. In the case that the (local) material is, in addition, isotropic in its reference configuration, it is well-established that the expression governing the energy storage of the elasto-plastic material can be reduced to an isotropic function $W = W(C, C_p)$, where $C = F^TF$ and $C_p = F_p^TF_p$, together with an isotropic flow rule for $C_p$, see eg. [12]. Here, $F_p$ itself does not appear anymore.

**Remark 2.1 (Why invariance 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 explicitely through the use of a corresponding invariant framework or structural tensors reflecting the given material symmetries [12]. If this is not done but the formulation is not fully rotationally form-invariant then one introduces inconsiderate anisotropic behaviour which lacks any real physical basis, cf. [13, p.220].*

### 2.2 The Plastic Indifference of the Elastic Response

In this work I concentrate on the hyperelastic formulation of finite strain plasticity, i.e., I am concerned with finding the appropriate energy storage terms governing the elastic and plastic behaviour. Moreover, I restrict attention to materials which are homogeneous in their purely elastic state.[2] In general, I assume then that the total stored energy can be expressed as a sum (this is already a constitutive assumption)

$$W(F, F_p, {\rm Curl}\,F_p) = \underbrace{W_{\rm e}(F, F_p)}_{\text{elastic energy}} + \underbrace{W_{\rm ph}(F_p)}_{\text{linear kinematical hardening}} + \underbrace{W_{\rm curl}(F_p, {\rm Curl}\,F_p)}_{\text{dislocation processes}}\,. \tag{4}$$

Here, the local hardening potential $W_{\rm ph}$ is a purely phenomenological energy storage term formally consistent with a Prager type constant linear hardening behaviour. The dislocation potential $W_{\rm curl}$ instead is a microscopically motivated energy storage term due to dislocation processes which is the ultimate physical reason for any hardening behaviour. It acts on ${\rm Curl}\,F_p$ which is the curl applied to the rows of $F_p$.

An additional constitutive assumption in finite strain plasticity is the plastic indifference[3] condition [17]. Plastic indifference implies that the elastic response of the material, governed by the elastic strain energy part, is invariant w.r.t. arbitrary previous plastic deformation $F_p^0$ [23]. This means that

$$\forall\, F_p \in GL^+(3): \quad W_{\rm e}(F, F_p) = W_{\rm e}(FF_p^0, F_pF_p^0)\,. \tag{5}$$

Using (5) it is easily seen, by specifying $F_p^0 = F_p^{-1}$, that

$$W_{\rm e}(F, F_p) = W_{\rm e}(FF_p^{-1}, \mathbb{1}) = W_{\rm e}(F_e)\,. \tag{6}$$

[1] The split is, formally, also invariant under any invertible $B(x) \in {\rm GL}^+(3)$ in the sense that $F = F_e\,F_p = F_e\,B^{-1}\,B\,F_p = F_e^\sharp\,F_p^\sharp$, but $F_e^\sharp$ leads to a different elastic response and cannot be considered as "equivalent" to $F_e$.

[2] No further $x$-dependence in (4): the material behaviour is the same in all material points.

[3] Conceptually similar is the assumption of **isomorphic elastic ranges** as discussed in [1]. The restrictive assumption of isomorphic elastic ranges fits well for aluminium but not really for copper.

Thus plastic indifference is a constitutive statement about the elastic response and not a fundamental physical invariance law. Plastic indifference reduces the effective elastic dependence of $W_{\rm e}$ on $F_e$ alone. It is based on the experimental evidence for some materials that unloading and consecutive loading below the yield limit has the same elastic response as the initial virgin response.

Remaining in the context of finite strain plasticity, I propose, following Bertram [1] a model based on evolution equations for $F_p$ and not on a plastic metric $C_p = F_p^T F_p$. In order to adapt the micromechanically motivated multiplicative decomposition to a description on the continuum level, one usually includes an assumption on the plastic spin, i.e., $\mathrm{skew}(F_p \frac{\rm d}{{\rm d}t} F_p^{-1}) = 0$, a no-spin multiplicative plasticity model based on $F_p$ results but I will retain from imposing such a condition.

Many of the existing gradient plasticity theories do not involve plastic rotations either, however, Gurtin/Anand [6] 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."

### 2.3 Illustration of the Phenomenological Multiplicative Decomposition Based on the Chain Rule

For illustration purposes let us introduce symbolically a compatible reference configuration $\Omega_{\rm ref}$, a fictitious compatible intermediate configuration $\Omega_{\rm int}$ and a compatible deformed configuration $\Omega_{\rm act}$, together with mappings

$$\begin{aligned} &\Psi_p : x \in \Omega_{\rm ref} \subset \mathbb{E}^3 \mapsto \Psi_p(\Omega_{\rm ref}) = \Omega_{\rm int} \subset \mathbb{E}^3\,, \quad \Psi_e : \eta \in \Omega_{\rm int} \subset \mathbb{E}^3 \mapsto \Omega_{\rm act} \subset \mathbb{E}^3\,, \\ &\varphi : x \in \Omega_{\rm ref} \subset \mathbb{E}^3 \mapsto \Omega_{\rm act} \subset \mathbb{E}^3\,, \\ &\varphi(x) = \Psi_e(\Psi_p(x))\,, \quad \nabla_x \varphi(x) = \nabla_\eta \Psi_e(\Psi_p(x))\, \nabla_x \Psi_p(x) = F_e(x)\, F_p(x)\,. \end{aligned} \tag{7}$$

This means that I assume to realize the total deformation $\varphi$ by two subsequent compatible deformations $\Psi_p$ and $\Psi_e$ and interprete $F_e$ and $F_p$ as the respective deformation gradients. A guiding question for this exposition can be stated as: *what form of constitutive restrictions are implied by respecting a possible gradient structure inherent in* (7). In this sense, this work extends the investigation in [3] from homogeneous deformations (suitable for the local situation without gradients on plastic variables ) to the inhomogeneous situation.

## 3 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[4] , moreover, it will turn out that the Prager linear kinematic hardening potential $W_{\rm ph}$ must be an isotropic function of $C_p = F_p^T F_p$. This conclusion can already be found in [3], for a recent account see [12, 11]. 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.,

$$W_{\rm e}(F_e\, \overline{Q}) = W_{\rm e}(F_e) \quad \forall\, \overline{Q} \in \mathrm{SO}(3)\,. \tag{8}$$

Concerning the determination of the plastic distortion $F_p$, following Maugin [15, p. 110], it should hold for referentially isotropic materials (nothing to do with isotropy w.r.t. the intermediate configuration) without gradients on the plastic distortion, that, comparing initial conditions

$$F_p(x,0) \quad \text{versus} \quad F_p(x,0)\, \overline{Q}^T\,, \tag{9}$$

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

$$F_p(x,t) \quad \text{versus} \quad F_p(x,t)\, \overline{Q}^T\,. \tag{10}$$

[4]The subsequent development shows that assuming form-invariance of the energy with respect to superposed rotations on the intermediate configuration already implies elastic isotropy.

For full isotropy w.r.t. the reference configuration the material symmetry group is $\mathrm{SO}(3)$. We note that the "plastic distortion rate" $F_p \, \frac{\mathrm{d}}{\mathrm{dt}}[F_p^{-1}]$ is form-invariant under $F_p \to F_p \, \overline{Q}^T$, thus the use of this rate is consistent with the requirement (10). It remains then to show that the energy related parts of the model will satisfy a suitably extended version of (10), taking also plastic gradients into account.

I refer to referential isotropy[5] if the model is form-invariant under the transformation

$$(F, F_e, F_p) \to (F\overline{Q}, F_e, F_p\overline{Q}) \,, \tag{11}$$

that means 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, where the rotation $\overline{Q}$ is understood to be one and the same rigid rotation of the whole body. 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

$$W_{\mathrm{ph}}(F_p\overline{Q}) = W_{\mathrm{ph}}(F_p) \quad \forall\, \overline{Q} \in \mathrm{SO}(3) \quad \Rightarrow \quad W_{\mathrm{ph}}(F_p) = \widehat{W}_{\mathrm{ph}}(F_pF_p^T) \,, \tag{12}$$

which can be seen by considering the left polar decomposition of $F_p = \sqrt{F_pF_p^T}\, R_p$ and specifying $\overline{Q} = R_p^T$.

In order to motivate the restrictions of referential isotropy for the gradient plasticity model I present a basic observation valid for homogeneous, isotropic hyperelasticity. In classical hyperelastic finite-strain elasticity isotropy (a priori now referential isotropy) can be viewed as a consequence of the form-invariance of the free-energy under a rigid rotation of the referential coordinate system. To see this consider the variational problem

$$\int_\Omega W(\nabla\varphi(x))\,\mathrm{dx} \mapsto \min \,. \quad \varphi \,, \tag{13}$$

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

$$\zeta : \Omega_{\mathrm{ref}} \mapsto \zeta(\Omega_{\mathrm{ref}}) = \Omega^* \,, \quad \zeta(x) = \xi \,. \tag{14}$$

By the transformation formula for integrals the problem (13) can be transformed to this new configuration. We define the same function $\varphi$ expressed in new coordinates (pull back of $\varphi$)

$$\varphi^*(\zeta(x)) := \varphi(x) \quad \Rightarrow \quad \nabla_\xi\varphi^*(\zeta(x))\,\nabla\zeta(x) = \nabla\varphi(x) \tag{15}$$

and consider

$$\int_{\xi\in\Omega^*} W(\nabla_\xi\varphi^*(\xi)\,\nabla_x\zeta(\zeta^{-1}(\xi)))\,|\mathrm{det}[\nabla_x\zeta^{-1}]|d\xi \mapsto \min \,. \quad \varphi^* \,. \tag{16}$$

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

$$W^*(\xi, \nabla_\xi\varphi^*(\xi)) = W(\nabla_\xi\varphi^*(\xi)\,\nabla_x\zeta(\zeta^{-1}(\xi)))\,|\mathrm{det}[\nabla_x\zeta^{-1}]| \,. \tag{17}$$

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

$$W^*(\nabla_\xi\varphi^*(\xi)) = W(\nabla_\xi\varphi^*(\xi)\,\overline{Q}) \,. \tag{18}$$

Now, in the classical hyperelastic context for homogeneous materials, isotropy is equivalent to form-invariance of $W$ under a rigid rotation of the referential coordinates, i.e.

$$W^*(X) \overbrace{=}^{\text{form-invariance}} W(X) \quad \Leftrightarrow \quad \forall\, \overline{Q} \in \mathrm{SO}(3) : \quad W(X\overline{Q}) \overbrace{=}^{\text{isotropy}} W(X) \,. \tag{19}$$

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

$$\Psi_p^*(\overline{Q}x) := \Psi_p(x) \quad \Rightarrow \quad \nabla_{x^*}\Psi_p^*(x^*)\,\overline{Q} = \nabla_x\Psi_p(x) \,. \tag{20}$$

[5] Papadopoulos [12] calls this "referential covariance" which is an extended statement of material symmetry relative to the given reference configuration.

This motivates to assume the transformation rule for $F_p$ under a rigid transformation of the reference configuration as being given as

$$F_p^*(x^*) = F_p^*(\overline{Q}x) = F_p(x)\,\overline{Q}^T\,. \tag{21}$$

Note that the argument of $F_p^*$ must also be changed accordingly.

It is not immediately obvious what type of transformation law for $\mathrm{Curl}\,F_p$ is induced under the transformation $F_p(x) \mapsto F_p(x)\overline{Q}^T$, even for constant rotations, since

$$\mathrm{Curl}_{\mathrm{x}}[F_p(x)\,\overline{Q}^T] \neq [\mathrm{Curl}_{\mathrm{x}}\,F_p(x)]\,\overline{Q}^T\,. \tag{22}$$

On the other hand it is simple to consider the transformation $F_p(x) \mapsto \overline{Q}\,F_p(x)$ and to deduce the corresponding transformation law $\mathrm{Curl}\,F_p \mapsto \overline{Q}\;\mathrm{Curl}\,F_p$, since

$$\mathrm{Curl}_{\mathrm{x}}[\overline{Q}\,F_p(x)] = \overline{Q}\,[\mathrm{Curl}_{\mathrm{x}}\,F_p(x)]\,. \tag{23}$$

Nevertheless, using the transformation law (21) for $F_p$ we are in a position to extend the invariance condition (10) also to include plastic gradients: for referential isotropy I postulate the form-invariance of the energy storage terms under a rigid rotation of the referential coordinates. First, for the local hardening contribution $W_{\mathrm{ph}}$ we have, from the transformation of integral formula

$$\int_{\xi\in\Omega^*} W_{\mathrm{ph}}(F_p^*(\xi)\overline{Q})\,\det[Q^T]d\xi\,, \tag{24}$$

such that

$$W_{\mathrm{ph}}^*(F_p^*(\xi)) := W_{\mathrm{ph}}(F_p^*(\xi)\overline{Q})\,, \tag{25}$$

and form-invariance demands that

$$W_{\mathrm{ph}}^*(X) = W_{\mathrm{ph}}(X) \quad \Rightarrow \quad \forall\,\overline{Q}\in\mathrm{SO}(3):\;\; W_{\mathrm{ph}}(X\overline{Q}) = W_{\mathrm{ph}}(X)\,, \tag{26}$$

which coincides with the result already obtained in (12).

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

$$\int_{\xi\in\Omega^*} W_{\mathrm{curl}}(F_p^*(\xi)\overline{Q}, \mathrm{Curl}_{\mathrm{x}}[F_p^*(\xi)\overline{Q}])\,\det[Q^T]d\xi\,, \tag{27}$$

such that

$$W_{\mathrm{curl}}^*(F_p^*(\xi), \mathrm{Curl}_{\xi}[F_p^*(\xi)]) := W_{\mathrm{curl}}(F_p^*(\xi)\overline{Q}, \mathrm{Curl}_{\mathrm{x}}[F_p^*(\xi)\overline{Q}])\,. \tag{28}$$

From a lengthy calculation in indicial notation, it holds[6]

$$\mathrm{Curl}_{\mathrm{x}}[F_p^*(\overline{Q}x)\,\overline{Q}]) = [\mathrm{Curl}_{\xi}\,F_p^*(\xi)]\,\overline{Q}\,, \tag{29}$$

which leads to

$$W_{\mathrm{curl}}^*(F_p^*(\xi), \mathrm{Curl}_{\xi}[F_p^*(\xi)]) := W_{\mathrm{curl}}(F_p^*(\xi)\overline{Q}, [\mathrm{Curl}_{\xi}\,F_p^*(\xi)]\,\overline{Q})\,. \tag{30}$$

Form-invariance for the dislocation energy storage demands therefore that

$$W_{\mathrm{curl}}^*(X,Y) = W_{\mathrm{curl}}(X,Y) \quad \Rightarrow\; W_{\mathrm{curl}}(X\overline{Q}, Y\overline{Q}]) = W_{\mathrm{curl}}(X,Y) \quad \forall\,\overline{Q}\in\mathrm{SO}(3)\,, \tag{31}$$

which is satisfied e.g., for $W_{\mathrm{curl}}(X,Y) = \|X^{-1}Y\|^2$. [7]

[6] The $(1,1)$-component in the matrix from the left hand side of (29) is equal to

$$\frac{\partial}{\partial x_2}(F_p^*)^1_k(\overline{Q}x)\overline{Q}^k_3 - \frac{\partial}{\partial x_3}(F_p^*)^1_k(\overline{Q}x)\overline{Q}^k_2 = \frac{\partial}{\partial\xi_l}(F_p^*)^1_k(\xi)[\overline{Q}^l_2\overline{Q}^k_3 - \overline{Q}^l_3\overline{Q}^k_2]\,.$$

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

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

which is the $(1,1)$-component of the matrix from the right hand side of (29). The proof for the other components is similar.

[7] Also satisfied for $\|Y\,X^T\|^2$ leading to a dislocation energy storage of the form $\|[\mathrm{Curl}\,F_p(x)]F_p^T(x)\|^2$, cf. (47).

## 4 Simultaneous Rigid Rotation of the Material and Spatial Coordinates

Let the reference configuration $\Omega_{\rm ref}$ be rigidly rotated through one constant rotation $Q_2 \in {\rm SO}(3)$. We let $\Omega^*_{\rm ref} = Q_2 \cdot \Omega_{\rm ref}$ together with the rotated coordinates $x^* = Q_2.x$. 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

$$\varphi^*(x^*) = Q_1\,\varphi(x) \quad \text{i.e.} \quad \Leftrightarrow\ \varphi^*(Q_2.x) = Q_1.\varphi(x)\,, \quad \forall\, x \in \Omega_{\rm ref}\,, \tag{32}$$

whether or not the material response is isotropic.[8] From (32) we obtain from the chain rule

$$\begin{aligned}\nabla_x[\varphi^*(x^*)] = \nabla_x[Q_1\,\varphi(x)] \ \Leftrightarrow\ \nabla_x[\varphi^*(Q_2.x)] = Q_1\nabla_x\varphi(x) \ \Leftrightarrow\ \nabla_{x^*}[\varphi^*(x^*)]\,Q_2 = Q_1\,\nabla_x\varphi(x)\\ Q_1^T\,\nabla_{x^*}[\varphi^*(x^*)]\,Q_2 = \nabla_x\varphi(x)\,.\end{aligned} \tag{33}$$

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

$$\begin{aligned}&W^*(F^*) = W^*(\nabla_{x^*}\varphi^*(x^*)) = W^*(Q_1\,\nabla\varphi(x)Q_2^T) := W(\nabla\varphi(x)) \ \Rightarrow\\ &W^*(F^*) = W(Q_1^T F^* Q_2)\,.\end{aligned} \tag{34}$$

This identity is used to define the rotated energy. If $W$ happens to be material frame-infifferent[9] and isotropic, i.e., form-invariant w.r.t. left and right multiplication by (not necessarily equal) constant rotation matrices (material and spatial form-invariance under rigid rotations), then $W(Q_1^T X Q_2) = W(X)$ and from (34) follows

$$W^*(X) = W(X)\,, \tag{35}$$

which is the desired form-invariance in case of purely elastic behaviour.

We now repeat the transformation under rigid rotations for each function appearing in (7) separately, i.e., it follows

$$\begin{aligned}&\Psi_p^*(Q_2^p.x) = Q_3^p\Psi_p(x) \ \Rightarrow \qquad Q_3^{p,T}\,\nabla_{x^*}[\Psi_p^*(x^*)]\,Q_2^p = \nabla_x\Psi_p(x)\,,\\ &\Psi_e^*(Q_3^e.\eta) = Q_1^e\Psi_e(\eta) \ \Rightarrow \qquad Q_1^{e,T}\,\nabla_{\eta^*}[\Psi_e^*(\eta^*)]\,Q_3^e = \nabla_\eta\Psi_e(\eta)\,,\\ &\varphi^*(Q_2.x) = Q_1\varphi(x) \ \Rightarrow \qquad Q_1^T\,\nabla_{x^*}[\varphi^*(x^*)]\,Q_2 = \nabla_x\varphi(x)\,.\end{aligned} \tag{36}$$

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

$$\begin{aligned}\varphi^*(x^*) &= Q_1\,\varphi(x) = Q_1\,\Psi_e(\Psi_p(x)) = Q_1\,\Psi_e(Q_3^T\,\Psi_p^*(x^*))\\ &= Q_1\,\left[Q_1^T\,\Psi_e^*(Q_3\,\left[Q_3^T\,\Psi_p^*(x^*)\right])\right] = \Psi_e^*(\Psi_p^*(x^*))\,,\end{aligned} \tag{37}$$

which implies

$$\nabla_{x^*}\varphi^*(x^*) = \nabla_{\eta^*}\Psi_e^*(\Psi_p^*(x^*))\,\nabla_{x^*}\Psi_p^*(x^*)\,, \quad F^*(x^*) = F_e^*(\eta^*)\,F_p^*(x^*)\,. \tag{38}$$

This suggests to identify

$$F_e^*(\eta^*) = \nabla_{\eta^*}\Psi_e^*(\Psi_p^*(x^*))\,, \quad F_p^*(x^*) = \nabla_{x^*}\Psi_p^*(x^*)\,. \tag{39}$$

However,

$$\begin{aligned}Q_1\,\nabla\varphi(x)\,Q_2^T &= Q_1\,\nabla_\eta\Psi_e(\Psi_p(x))\,\nabla_x\Psi_p(x)\,Q_2^T = Q_1\,\nabla_\eta\Psi_e(\Psi_p(x))\,Q_3^T\,Q_3\,\nabla_x\Psi_p(x)\,Q_2^T\\ Q_1\,F(x)\,Q_2^T &= Q_1\,F_e(x)\,Q_3^T\,\left(Q_3\,F_p(x)\,Q_2^T\right) = Q_1\,F_e(x)\,F_p(x)\,Q_3^T\,,\end{aligned} \tag{40}$$

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

$$\underbrace{Q_1\,F(x)\,Q_2^T}_{=F^*(x^*)} = Q_1\,F_e(x)Q_3^T\,Q_3\,F_p(x)\,Q_2^T = \underbrace{Q_1\,F_e(x)\,Q_3^T}_{=:F_e^*(\eta^*)}\ \underbrace{(Q_3\,F_p(x)\,Q_2^T)}_{=F_p^*(x^*)}\,, \tag{41}$$

[8] For homogeneous 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.

[9] See [22, 2] for an in depth discussion of the different concepts subsumed in the not precisely defined term "objectivity".

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

Hence we conclude that under a rigid rotation of the reference configuration and simultaneous rotation of the intermediate and spatial coordinates the following obtains

$$\begin{aligned} F^*(x^*) &= Q_2\, F(x)\, Q_1^T\,, \qquad F_e^*(\eta^*) = Q_1\, F_e(\eta)\, Q_3^T\,, \\ F_p^*(x^*) &= Q_3\, F_p(x)\, Q_1^T = Q_3\, F_p(Q_2^T x^*)\, Q_1^T\,. \end{aligned} \tag{42}$$

Since such changes of coordinates leave the composition of mappings invariant I require that the model be form-invariant under these transformations. I refer to this as elasto-plastic transformation invariance requirement.[10] Note that the postulated transformation law (42) for the multiplicative decomposition is not meant to read:

$$\begin{aligned} &F(x) = F_e(x)F_p(x) \;\Rightarrow Q_1(x)F(x)Q_2(x)^T = Q_1(x)F_e(x)Q_3^T(x)Q_3(x)F_p(x)Q_2(x)^T \;\Rightarrow \\ &F(x) = F_e(x)Q_3^T(x)Q_3(x)F_p(x) = F_e^*(x)\,F_p^*(x)\,, \end{aligned} \tag{43}$$

for all non-constant rotations $Q_{1,2,3}(x) \in \mathrm{SO}(3)$ since this would destroy compatibility. Requiring (43) would reduce the theory (including higher gradients) necessarily to a model based only on the plastic metric $C_p(x) = F_p^T(x)F_p(x)$ and a compatibility measure for $C_p$ as gradient contribution. The much more restrictive condition (43) is sometimes motivated by the observation that the multiplicative split is locally unique only up to a local rotation $Q_3(x) \in \mathrm{SO}(3)$, which, viewed without compatibility requirements, is self-evident. It has already been observed by Casey/Naghdi [3, Eq.(13)] that full local "objectivity"-requirements on the multiplicative decomposition (i.e., to allow non-constant rotation matrices in (42)) reduces the model to an isotropic formulation in $C = F^TF$ and $C_p = F_p^TF_p$. Our development, however, shows that this conclusion is strictly constraint to the local theory without gradients on the plastic distortion: the local theory simply cannot distinguish between local rotations and global rigid rotations.

For a fully rotationally form-invariant model the form-invariant transformation behaviour of the elastic energy (35) under (42) will be postulated for all contributions separately, i.e., for all constant $Q_{1,2,3} \in \mathrm{SO}(3)$ it must be satisfied

$$\begin{aligned} W_{\mathrm{e}}^*(X) &:= W_{\mathrm{e}}(Q_1^T X Q_3) = W_{\mathrm{e}}(X)\,, \\ W_{\mathrm{ph}}^*(X) &:= W_{\mathrm{ph}}(Q_3^T X Q_2) = W_{\mathrm{ph}}(X)\,, \\ W_{\mathrm{curl}}^*(X, \mathrm{Curl}_\xi\, X) &:= W_{\mathrm{curl}}(Q_3^T X Q_2, \mathrm{Curl}_x[Q_3^T X Q_2]) \\ &\qquad = W_{\mathrm{curl}}(Q_3^T X Q_2, Q_3^T[\mathrm{Curl}_\xi\, X]Q_2]) = W_{\mathrm{curl}}(X, \mathrm{Curl}_\xi\, X)\,, \\ W_{\mathrm{curl}}(Q_3^T X Q_2, Q_3^T Y Q_2]) &= W_{\mathrm{curl}}(X, Y)\,. \end{aligned} \tag{44}$$

Thus $W_{\mathrm{e}}$ and $W_{\mathrm{ph}}$ must be isotropic and frame-indifferent functions of their arguments which is easily met whenever the functional dependence can be reduced to isotropic functions of $C_e = F_e^TF_e$ and $C_p = F_p^TF_p$. A sufficient condition for $W_{\mathrm{curl}}$ to satisfy (44) is given e.g., by taking

$$\begin{aligned} &W_{\mathrm{curl}}(X, Y) = \mathcal{H}(X^{-1}Y) \quad \text{or} \quad \mathcal{H}(X^TY) \quad \text{with} \\ &\mathcal{H}(Q^TZQ) = \mathcal{H}(Z) \quad \forall\, Q \in \mathrm{SO}(3)\,. \end{aligned} \tag{45}$$

For the remainder I choose $\mathcal{H}(Z) = \|Z\|^2$ and $Z = X^{-1}Y$.

## 5 A Form-Invariant Finite Strain Thermodynamic Potential

We have arrived at postulating the invariance of the plasticity model according to (42) and (35). To be specific let us write down a modified Saint-Venant Kirchhoff isotropic quadratic energy $W_{\mathrm{e}}$ in the elastic stretches $F_e^TF_e$,

[10] It 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 the stress free reference configuration of the curved shell.

augmented with local self-hardening $W_{\rm ph}$ and a contribution accounting for plastic gradients $W_{\rm curl}$

$$W(F_e,F_p,\operatorname{Curl}F_p)=W_{\rm e}(F_e)+W_{\rm ph}(F_p)+W_{\rm curl}(F_p,\operatorname{Curl}F_p)\,, \tag{46}$$
$$W_{\rm e}(F_e)=\frac{\mu}{4}\|\frac{F_e^TF_e}{\det[F_e]^{2/3}}-\mathbb{1}\|^2+\frac{\lambda}{4}\left((\det[F_e]-1)^2+(\frac{1}{\det[F_e]}-1)^2\right),$$
$$W_{\rm ph}(F_p)=\frac{\mu\,h^+}{4}\|\frac{F_p^TF_p}{\det[F_p]^{2/3}}-\mathbb{1}\|^2\,,\quad W_{\rm curl}(F_p,\operatorname{Curl}F_p)=\frac{\mu\,L_c^2}{2}\,\|F_p^{-1}\operatorname{Curl}F_p\|^2\,.$$

Note that in this setting $F_p$ is not needed to be volume preserving. Here, $\mu,\lambda$ 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 form-invariant and satisfies the plastic indifference condition. The elastic energy $W_{\rm e}$ is additively decoupled into a volumetric and isochoric contribution, it is frame-indifferent and isotropic w.r.t. the intermediate configuration. The term $W_{\rm ph}$ accounts for phenomenological local plastic hardening in the spirit of Prager constant linear hardening. It is fully form-invariant and indifferent to plastic volume changes. The term $W_{\rm curl}$ represents energy storage due to dislocations. Its argument $G_{\rm R}=F_p^{-1}\operatorname{Curl}F_p$ is the referential version of the tensor $G=\frac{1}{\det[F_p]}(\operatorname{Curl}F_p)F_p^T$, 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 [5, 20]. It transforms as $G(QF_p)=QG(F_p)Q^T$ for all rigid rotations $Q$. This tensor introduces the influence of **g**eometrically (kinematically) **n**ecessary **d**islocations (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 $\sigma$, which satisfies as well the invariances $\forall\ Q\in{\rm SO}(3):\ \sigma(QF)=Q\sigma(F)Q^T$. Note that our corresponding referential measure $G_{\rm R}$ [5, Eq.(6.1)] is given by

$$G_{\rm R}=F_p^{-1}\operatorname{Curl}F_p\,,\quad G=\frac{1}{\det[F_p]}(\operatorname{Curl}F_p)F_p^T=\frac{1}{\det[F_p]}\,F_p\,G_{\rm R}\,F_p^T\,. \tag{47}$$

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

$$F(x)=F_e(x)F_p(x)=F_e(x)\overline{B}^{-1}\overline{B}F_p(x)=\tilde{F}_e(x)\,\tilde{F}_p(x)\,,$$
$$G_{\rm R}(\overline{B}F_p(x))=G_{\rm R}(F_p(x))\,,\quad\forall\,\overline{B}\in{\rm GL}^+(3)\,, \tag{48}$$

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

In order to close the model it remains to motivate a flow rule for $F_p$. Relevant in this respect are the thermodynamical driving forces acting on the internal variable $F_p$. These driving forces now necessarily include second space derivatives of $F_p$. The evolution equation for $F_p$ is coupled in space to the balance of forces equation. This constitutes a significant difficulty as compared to the classical local evolution equations.

## 6 Discussion

Many other problems are still in need of investigation. We have not treated the question of how boundary values for $F_p$ should be prescribed and on what reasoning this should be based. A tentative answer has been given in [18]. There, also the mathematical questions of existence and uniqueness of a linearization of the present model is addressed.

Here, attention is restricted to a formulation of the thermodynamic potential. This is done in a finite-strain setting based on the multiplicative decomposition. I apply a strict principal of referential, intermediate and spatial form-invariance under rigid rotations. Referential form-invariance severely restricts the choice of the hardening contribution. However, full form-invariance w.r.t. constant rotations does not reduce the gradient plasticity model to a dependence on the plastic metric $C_p=F_p^TF_p$, in contrast to the classical case without gradients on the plastic distortion. In this context the gradient plasticity model allows to distinguish in more detail between form-invariance under all rotations (form-invariance for the local model) and form-invariance under rotations constant over the body (form-invariance for the 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 form-invariance with respect to rigid rotations of the reference, intermediate and spatial configuration in the multiplicative decomposition the model should satisfy the comprehensive condition (44).

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## Notation

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

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