

A fourth-order gauge-invariant gradient plasticity model for polycrystals based on Kröner's incompatibility tensor

François Ebobisse 

Department of Mathematics and Applied Mathematics, University of Cape Town, South Africa

Patrizio Neff

Faculty of Mathematics, University of Duisburg-Essen, Germany

Received 24 April 2018; accepted: 25 March 2019

Abstract

In this paper we derive a novel fourth-order gauge-invariant phenomenological model of infinitesimal rate-independent gradient plasticity with isotropic hardening and Kröner's incompatibility tensor $\text{inc}(\varepsilon_p) := \text{Curl}[(\text{Curl } \varepsilon_p)^T]$, where ε_p is the symmetric plastic strain tensor. Here, gauge-invariance denotes invariance under diffeomorphic reparametrizations of the reference configuration, suitably adapted to the geometrically linear setting. The model features a defect energy contribution that is quadratic in the tensor $\text{inc}(\varepsilon_p)$ and it contains isotropic hardening based on the rate of the plastic strain tensor $\dot{\varepsilon}_p$. We motivate the new model by introducing a novel rotational invariance requirement in gradient plasticity, which we call micro-randomness, suitable for the description of polycrystalline aggregates on a mesoscopic scale and not coinciding with classical isotropy requirements. This new condition effectively reduces the increments of the non-symmetric plastic distortion $\dot{\rho}$ to their symmetric counterpart $\dot{\varepsilon}_p = \text{sym } \dot{\rho}$. In the polycrystalline case, this condition is a statement about insensitivity to arbitrary superposed grain rotations. We formulate a mathematical existence result for a suitably regularized non-gauge-invariant model. The regularized model is rather invariant under reparametrizations of the reference configuration including infinitesimal conformal mappings.

Keywords

gradient plasticity, geometrically necessary dislocations, variational inequality, defect energy, incompatibility tensor, Riemann–Christoffel tensor, dislocation density, gauge theory of dislocations, infinitesimal conformal mappings, isotropy

1. Introduction

In recent years growing attention has been paid to extending continuum plasticity theories towards the incorporation of the experimentally observed size effects in small scales (see e.g. [1–4]). This extension is mainly done via the introduction of certain gradient terms, making the plastic evolution in some sense non-local. Perhaps the

Dedicated to Elias C. Aifantis, pioneer of gradient plasticity

Corresponding authors:

François Ebobisse, Department of Mathematics and Applied Mathematics, University of Cape Town, Rondebosch 7700, South Africa.

Email: francois.ebobissebille@uct.ac.za

Mathematics and Mechanics of Solids
2020, Vol. 25(2) 129–159

© The Author(s) 2019

Article reuse guidelines:

sagepub.com/journals-permissions

DOI: 10.1177/1081286519845026

journals.sagepub.com/home/mms



Table 1. Summary of the model by Aifantis et al. [5–7] based on the accumulated equivalent plastic strain γ_p . Depending on the sign of $\Delta\gamma_p$, the model describes process-dependent hardening ($\Delta\gamma_p < 0$) or softening ($\Delta\gamma_p > 0$) owing to non-local effects.

$\text{sym } \nabla u = \varepsilon = \varepsilon_e + \varepsilon_p, \quad \varepsilon_p \in \text{Sym}(3)$ $\sigma_y = \sigma_0 + \mu k_2 \gamma_p - \mu L_c^2 \Delta\gamma_p, \quad \sigma_y \text{ is the current yield stress}$ $L_c > 0$ material length scale $\sigma_0 > 0$ the initial yield stress k_2 can be taken negative for local softening behaviour $\gamma_p := \int_0^t \ \dot{\varepsilon}_p\ ds$ the accumulated equivalent plastic strain.

earliest such phenomenological model is due to Aifantis et al. [5–8], [95–98] and [135, 136] who directly incorporated the Laplacian $\Delta\gamma_p$ in the flow stress, where $\gamma_p := \int_0^t \|\dot{\varepsilon}_p\| ds$ is a measure of accumulated equivalent plastic strain¹ (see Table 1 for a summary).

Other variants of the Aifantis model also based on the accumulated plastic strain were proposed later through the principle of virtual power by Fleck and Hutchinson [10], Gudmundson [11], and generalized by Gurtin and Anand [12].

While there are numerous proposals of such gradient enhanced phenomenological models, either based on the multiplicative decomposition

$$F = F_e \cdot F_p \quad (1)$$

(see e.g. [13–16]), or based on the geometrically linearized corresponding additive decomposition

$$\varepsilon = \varepsilon_e + \varepsilon_p \quad (2)$$

(see e.g. [5–7, 10–12, 17–21], [100–103, 108–109, 113]), no general consensus has been reached as to which variables describing the plastic evolution should be employed and how they should be combined with their partial derivatives in space. For example, a dependence of the plastic flow rule directly via the infinitesimal plastic strain variable ε_p is sometimes excluded, because the backstress variable ε_p is not *gauge-invariant*.²

However, if ε_p is not allowed to appear itself in the equations, then linear kinematic hardening á la Prager is excluded from the onset, whereas the modelling of classical linear isotropic hardening remains possible because it is based on $\|\dot{\varepsilon}_p\|$, which is invariant under reparametrization of the reference configuration (*gauge-invariance*), see Section 3.1 in this paper.

With the use of an evolution equation for the symmetric plastic strain tensor ε_p being traditional, there are also approaches that focus directly on the plastic distortion p (which is a non-symmetric variable), thus allowing for the so-called *plastic spin*³ (see [22, p. 493 and (91.7) and (91.10)] and also [23–28], [129]). The connection between the two approaches is simple: we can always identify $\varepsilon_p := \text{sym } p$. As it will turn out subsequently, the introduction of the plastic distortion p will make our modelling framework much more transparent: on the one hand, the passage from the multiplicative decomposition to the additive decomposition via formal geometric linearization is easier and the discussion of invariance conditions becomes clearer, even if in the end we obtain a model for the plastic strain tensor $\varepsilon_p = \text{sym } p$ only.

Our aim with this paper is to present a rational modelling environment for gradient plasticity with respect to the small strain framework and the additive decomposition which incorporates certain insights learned from the multiplicative decomposition.

Let us therefore collect what the model should be able to do. It should:

- incorporate energetic hardening (owing to geometrically necessary dislocations (GNDs)) related to the energetic length scale L_c ;
- incorporate non-local hardening (backstress and Bauschinger effects);
- satisfy appropriate invariance conditions (objectivity, referential isotropy, independence of reference configuration, gauge-invariance, elastic isotropy, elastic frame-indifference, etc.);
- allow, in principle, for plastic spin [16, 26, 29–33]);
- satisfy an extended positive dissipation principle and therefore be thermodynamically admissible;
- be able to be cast in a convex analytical framework;
- support a well-posedness result in both the rate-independent and the rate-dependent cases;

- have physical meaningful and transparent boundary conditions for the plastic variables.

In this paper, we propose such a model, which, in the end, has a certain resemblance with the early model proposed by Menzel and Steinmann [20] and we show its well-posedness in the rate-independent case with a suitable regularization. Our derivation of the model based on invariance principles is, to the best of the authors' knowledge, entirely new. The model is derived through a process of linearization of some state variables in the finite strain case. The derivation of a linear model from a finite strain one is not new in the context of elasto-plasticity. For instance, Mielke and Stefanelli [34] used Γ -convergence to derive rigorously a model of linearized plasticity as the limit of some finite strain plasticity model.

The mathematical well-posedness of our model seems to be interesting in its own right. Once more, the convex analytical framework, based on incorporating the postulate of maximum plastic dissipation (PMDP),⁴ put forward initially by Moreau [39] and used later by many authors (e.g. [16, 31–33, 40–45]), proves to be ideally suited. For that purpose, our “additive” model also admits a finite strain parent model by Krishnan and Steigmann [46], who did not consider, however, the incorporation of (non-local) kinematic hardening.

Decisive for our new strain gradient plasticity model is the introduction of Kröner's incompatibility tensor inc (see [47–52], [118]) as an inhomogeneity measure acting on the symmetric plastic strain $\varepsilon_p = \text{sym } p$. This *incompatibility tensor* is given by

$$\text{inc}(\text{sym } p) := \text{Curl}([\text{Curl } \text{sym } p]^T) \quad (3)$$

and it coincides to first order with the Riemann–Christoffel curvature tensor \mathcal{R} in the metric characterized by the finite plastic strain tensor $C_p := F_p^T F_p$ (De Wit [53]). In fact, considering the non-symmetric plastic distortion F_p in the multiplicative decomposition (1) and writing $F_p = \mathbb{1} + p$, the connection is

$$\mathcal{R}(F_p^T F_p) = \mathcal{R}((\mathbb{1} + p)^T (\mathbb{1} + p)) = \mathcal{R}(\mathbb{1} + 2 \text{sym } p + p^T p) = 2 \text{inc}(\text{sym } p) + \text{h.o.t.}, \quad (4)$$

where⁵

$$\mathcal{R}_{jkl}^i(C_p) := \frac{\partial \Gamma_{jl}^i}{\partial x_k} - \frac{\partial \Gamma_{jk}^i}{\partial x_l} + \Gamma_{jl}^m \Gamma_{mk}^i - \Gamma_{jk}^m \Gamma_{ml}^i, \quad (5)$$

with

$$\Gamma_{ij}^l := \frac{1}{2} g^{kl} \left[\frac{\partial g_{ki}}{\partial x_j} + \frac{\partial g_{jk}}{\partial x_i} - \frac{\partial g_{ij}}{\partial x_k} \right]$$

being the Christoffel symbols of the second kind in the metric $C_p = (g_{ij})$ whose inverse is $C_p^{-1} = (g^{ij})$.

Assume that we change the reference configuration by a smooth invertible map

$$\psi : \xi \mapsto x(\xi), \quad (6)$$

then the plastic distortion F_p in the multiplicative decomposition (1) should transform according to

$$F_p(x) \longrightarrow F_p(x(\xi)) \frac{\partial x(\xi)}{\partial \xi} = \tilde{F}_p(\xi) \nabla_\xi \psi(\xi). \quad (7)$$

Based on the Riemann–Christoffel curvature tensor \mathcal{R} in (5), we may form a “true scalar” quantity, namely the so-called *Lanczos scalar*

$$\sum_{ijkl} \mathcal{R}_{jkl}^i \cdot \mathcal{R}_{jkl}^i =: \|\mathcal{R}\|_{\mathbb{R}^{81}}^2, \quad (8)$$

which is *form-invariant* under a change of the reference configuration in the sense that

$$\|\mathcal{R}_x(F_p(x)^T F_p(x))\|^2 = \|\mathcal{R}_\xi((\tilde{F}_p(\xi) \nabla_\xi \psi(\xi))^T (\tilde{F}_p(\xi) \nabla_\xi \psi(\xi)))\|^2, \quad (9)$$

(see Lanczos [54, (2.3)]) where \mathcal{R}_x and \mathcal{R}_ξ denote the Riemann–Christoffel curvature tensor expressed in coordinates x and ξ , respectively. Moreover, if we consider the transformation

$$F_p(x) \longrightarrow \hat{F}_p := Q(x) F_p(x), \quad \text{with arbitrary } Q(x) \in \text{O}(3), \quad (10)$$

then we have the direct invariance condition for the Riemann–Christoffel curvature tensor

$$\begin{aligned}\mathcal{R}_x(F_p(x)^T F_p(x)) &= \mathcal{R}_x(F_p(x)^T Q(x)^T Q(x) F_p(x)) = \mathcal{R}_x((Q(x) F_p(x))^T Q(x) F_p(x)) \\ &= \mathcal{R}_x(\widehat{F}_p(x)^T \widehat{F}_p(x)).\end{aligned}\quad (11)$$

The form-invariance property (9) is inherited in its geometric linearization, now by the inc-operator, in the form of a direct invariance condition for the complete operator (and not just the “Lanczos”-type scalar $\|\text{inc}_x \text{sym } p\|^2$):

$$\text{inc}_x(\text{sym } p(x)) = \text{inc}_x(\text{sym}(p(x) + \nabla_x \vartheta(x))) \quad \forall \vartheta(x) \in C^\infty(\mathbb{R}^3, \mathbb{R}^3), \quad (12)$$

where we have identified $\psi(x) = x + \vartheta(x)$. In fact, from the identity (see [55, Proposition 2.1])

$$\nabla \text{axl}(\text{skew } \nabla \vartheta) = \frac{1}{2} \nabla \text{curl } \vartheta = (\text{Curl } \text{sym } \nabla \vartheta)^T, \quad (13)$$

taking the Curl on both sides, we obtain

$$0 = \text{Curl} \left(\frac{1}{2} \nabla \text{curl } \vartheta \right) = \text{Curl} [(\text{Curl } \text{sym } \nabla \vartheta)^T] = \text{inc}(\text{sym } \nabla \vartheta), \quad (14)$$

which shows (12). Of course (12) implies that

$$\|\text{inc}_x(\text{sym } p(x))\|^2 = \|\text{inc}_x(\text{sym}(p(x) + \nabla_x \vartheta(x)))\|^2 \quad \forall \vartheta(x) \in C^\infty(\mathbb{R}^3, \mathbb{R}^3), \quad (15)$$

mirroring property (9) for the Lanczos-type scalar.

In addition, the direct invariance condition (11) for \mathcal{R} under rotation fields $Q(x) \in \text{SO}(3)$ translates to an invariance condition on the inc-operator as well. We write $Q(x) = \mathbb{1} + A(x) + \text{h.o.t.}$ with $A(x) \in \mathfrak{so}(3)$ and in terms of the infinitesimal plastic distortion, we consider

$$p(x) \longrightarrow A(x) + p(x) \quad \forall A(x) \in \mathfrak{so}(3)$$

and we have the invariance condition

$$\text{inc}_x(\text{sym } p(x)) = \text{inc}_x(\text{sym}(A(x) + p(x))) \quad \forall A(x) \in \mathfrak{so}(3). \quad (16)$$

For both tensors \mathcal{R} and inc we note the Saint-Venant compatibility condition and its linearization:

$$\boxed{\psi(x) = x + \vartheta(x)} \quad \text{and} \quad \boxed{C_p = F_p^T F_p = \mathbb{1} + \varepsilon_p + \text{h.o.t.}} \quad (17)$$

$$C_p = F_p^T F_p \in \text{Sym}^+(3) \text{ symmetric positive definite}$$

$$\mathcal{R}(C_p) = 0 \Leftrightarrow C_p = \nabla \psi^T \nabla \psi$$

See e.g. Ciarlet-Laurent [56, Theorem 1.1]

$$\approx \boxed{\text{inc}(\text{sym } p) = 0 \Leftrightarrow \text{sym } p = \text{sym } \nabla \vartheta}$$

in simply connected domains (see [56–59]). For more properties of the inc-operator, we refer the reader to [50, 59, 60].

With these preliminaries, both tensors \mathcal{R} and inc qualify as incompatibility measures on positive-definite symmetric plastic strains $C_p = F_p^T F_p$ in the geometrically nonlinear and on symmetric plastic strains $\varepsilon_p = \text{sym } p$ in the geometrically linear settings, respectively.

In a purely phenomenological context, we have another way to measure the incompatibility of the plastic distortion F_p itself via the so-called *dislocation density tensor* $\text{Curl}_x F_p(x)$ (see for instance [15, 16]). Following the works of Davini and Parry [61], Cermelli and Gurtin [14] and Epstein [62], [125–128] it has been shown that the differential operator (the “true dislocation density tensor”)⁶

$$\frac{1}{\det F_p} (\text{Curl } F_p) F_p^T = \det F_e (\text{Curl}_C F_e^{-1}) F_e^{-T}, \quad (18)$$

Table 2. We need to realize that $\text{Curl } p$ is a “sharper” incompatibility measure than $\text{inc}(\text{sym } p)$.

$\begin{aligned} \text{Curl } p = 0 &\Rightarrow p = \nabla \vartheta \\ &\Rightarrow \text{inc}(\text{sym } p) = \text{inc}(\text{sym } \nabla \vartheta) = 0 \end{aligned}$	$\begin{aligned} \text{inc}(\text{sym } p) = 0 &\Rightarrow \text{sym } p = \text{sym } \nabla \vartheta \\ &\not\Rightarrow p = \nabla \vartheta \text{ but} \\ &\Rightarrow p = \nabla \vartheta + A(x), \quad A(x) \in \mathfrak{so}(3) \\ &\not\Rightarrow \text{Curl } p = 0 \end{aligned}$
---	--

(where Curl_C means taking the spatial Curl with respect to the current configuration) is also *form-invariant* under arbitrary coordinate transformation of the reference placement (see [14, (1.4) on p. 1542]).⁷ This property is easily understood from $(18)_2$, which is invariant under reparametrization of the reference system anyway.

From now on, we assume plastic incompressibility, i.e. $\det F_p = 1$ and $\text{tr } p = 0$. Either

$$(\text{Curl}_x F_p) F_p^T \text{ linearized through } F_p = \mathbb{1} + p \text{ turns into } \text{Curl}_x p \quad (19)$$

or

$$\mathcal{R}(F_p^T F_p) \text{ linearized through } F_p = \mathbb{1} + p \text{ turns into } \text{inc}(\text{sym } p). \quad (20)$$

Therefore, in the geometrically linear setting, two measures of incompatibility of the infinitesimal plastic distortion p are used in the literature. Some authors use the tensor $\text{Curl } p$ (see [16, 17, 64, 65]) while others use $\text{inc}(\text{sym } p)$ (see [20]). See Table 2.

Concerning the invariance of the curvature tensor \mathcal{R} observed in (9), we note that under a change of reference placement $F_p(x) \rightarrow \tilde{F}_p(\xi) \nabla \psi(\xi)$, we obtain directly the *form-invariance* of the true dislocation density tensor $(\text{Curl } F_p) F_p^T$ as well, meaning that

$$(\text{Curl}_x F_p) F_p^T = (\text{Curl}_\xi (\tilde{F}_p(\xi) \nabla \psi(\xi))) (\tilde{F}_p(\xi) \nabla \psi(\xi))^T, \quad (21)$$

where Curl_x and Curl_ξ are the Curl expressed in coordinates x and ξ , respectively. Therefore, the expression $\|(\text{Curl}_x F_p) F_p^T\|^2$ is also a true scalar quantity. Accordingly, in the linearized setting we consider as in (12)

$$p(x) \rightarrow p(x) + \nabla \vartheta(x) \quad (22)$$

and we obtain directly the invariance

$$\text{Curl } p(x) = \text{Curl} [p(x) + \nabla \vartheta(x)], \quad (23)$$

similar to (12).

Concerning superposition of rotation fields, we note that for $F_p \rightarrow \bar{Q} F_p$ for $\bar{Q} \in \text{O}(3)$ where \bar{Q} is a homogeneous rotation, we have

$$(\text{Curl}(\bar{Q} F_p)) (\bar{Q} F_p)^T = \bar{Q} (\text{Curl } F_p) F_p^T \bar{Q}^T. \quad (24)$$

Similarly, in the linearized setting we consider $p(x) \rightarrow \bar{A} + p(x)$ for every $\bar{A} \in \mathfrak{so}(3)$ with \bar{A} a constant skew-symmetric matrix and we obtain

$$\text{Curl } p(x) = \text{Curl} [\bar{A} + p(x)]. \quad (25)$$

We have the relation

$$\boxed{\psi(x) = x + \vartheta(x)} \quad \text{and} \quad \boxed{F_p = \mathbb{1} + p} \\ \boxed{(\text{Curl } F_p) F_p^T = 0 \Leftrightarrow F_p = \nabla \psi} \quad \equiv \quad \boxed{\text{Curl } p = 0 \Leftrightarrow p = \nabla \vartheta} \quad (26)$$

in simply connected domains and under appropriate regularity conditions (see [66, Section 59]).

The difference between the two incompatibility measures for the linearized setting, $\text{inc}(\text{sym } p)$ on the one hand and $\text{Curl } p$ on the other hand, is the invariance property under superposed infinitesimal rotations. While

$\text{inc}(\text{sym } p)$ allows to *superpose any inhomogeneous* infinitesimal rotation field $A(x)$, $\text{Curl } p$ allows to *superpose only homogeneous* infinitesimal rotation fields \bar{A} .

In single-crystal gradient plasticity, it is typically $\text{Curl } F_p$ which is used, whereas it is debatable whether $\text{Curl } F_p$ is a good state-variable for polycrystalline material without texture.

In the following, we use a set of invariance conditions that allow us to decide between using Curl or inc . It is clear, however, that assuming a set of invariance requirements is already a constitutive requirement and therefore subject to discussion.⁸ In all these developments, beyond the discussion on which invariance principles are applied, it is our aim to clearly state and show, which kind of modelling restrictions will be obtained from them.

Our contribution is structured as follows: after introducing in Section 2 some notation, operators and function spaces used throughout the paper, we set the stage in Section 3 with two important invariance conditions on which our model will be tested. Namely, the *gauge-invariance* known as invariance under compatible transformations of the reference system, and a novel rotational invariance postulate for polycrystals, called *micro-randomness*. In Section 4, we first present few models of gradient plasticity with Kröner's incompatibility tensor which fail our invariance conditions, then we introduce our novel fourth-order phenomenological model which, though it fails also the gauge-invariance condition, is invariant with respect to a subclass of reparametrizations of the reference configurations, including the infinitesimal conformal group. The new model is then formulated using the convex analytical framework leading to mathematical strong and weak formulations. Finally an existence result for the weak formulation is obtained in the same framework as in [40–45, 77, 78, 86, 113, 117].

Let us next fix some notation and definitions which will also make the paper more clear and readable.

2. Some notational agreements and definitions

Let Ω be a bounded domain in \mathbb{R}^3 with Lipschitz continuous boundary $\partial\Omega$, which is occupied by an elastoplastic body in its undeformed configuration. Let Γ be a smooth subset of $\partial\Omega$ with non-vanishing two-dimensional Hausdorff measure. A material point in Ω is denoted by x and the time domain under consideration is the interval $[0, T]$.

For every $a, b \in \mathbb{R}^3$, we let $\langle a, b \rangle_{\mathbb{R}^3}$ denote the scalar product on \mathbb{R}^3 with associated vector norm $\|a\|_{\mathbb{R}^3}^2 = \langle a, a \rangle_{\mathbb{R}^3}$. We denote by $\mathbb{R}^{3 \times 3}$ the set of real 3×3 tensors. The standard Euclidean scalar product on $\mathbb{R}^{3 \times 3}$ is given by $\langle A, B \rangle_{\mathbb{R}^{3 \times 3}} = \text{tr}[AB^T]$, where B^T denotes the transpose tensor of B . Thus, the Frobenius tensor norm is $\|A\|^2 = \langle A, A \rangle_{\mathbb{R}^{3 \times 3}}$. In the following, we omit the subscripts \mathbb{R}^3 and $\mathbb{R}^{3 \times 3}$. The identity tensor on $\mathbb{R}^{3 \times 3}$ will be denoted by $\mathbb{1}$, so that $\text{tr}(A) = \langle A, \mathbb{1} \rangle$. We let $\text{GL}(3) := \{X \in \mathbb{R}^{3 \times 3} \mid \det(X) \neq 0\}$ denote the group of invertible 3×3 square matrices; $\text{GL}^+(3) := \{X \in \mathbb{R}^{3 \times 3} \mid \det(X) > 0\}$; $\text{SO}(3) := \{X \in \text{GL}(3) \mid XX^T = \mathbb{1}, \det[X] = 1\}$ is the Lie group of rotations in \mathbb{R}^3 whose Lie algebra is the set $\mathfrak{so}(3) := \{X \in \mathbb{R}^{3 \times 3} \mid X^T = -X\}$ of skew-symmetric tensors. We let $\text{Sym}(3) := \{X \in \mathbb{R}^{3 \times 3} \mid X^T = X\}$ denote the set of symmetric tensors and $\mathfrak{sl}(3) := \{X \in \mathbb{R}^{3 \times 3} \mid \text{tr}(X) = 0\}$ be the Lie algebra of traceless tensors. For every $X \in \mathbb{R}^{3 \times 3}$, we set $\text{sym}(X) = \frac{1}{2}(X + X^T)$, $\text{skew}(X) = \frac{1}{2}(X - X^T)$ and $\text{dev}(X) = X - \frac{1}{3}\text{tr}(X)\mathbb{1} \in \mathfrak{sl}(3)$ for the symmetric part, the skew-symmetric part and the deviatoric part of X , respectively. Quantities which are constant in space will be denoted with an overbar, e.g., $\bar{A} \in \mathfrak{so}(3)$ for the function $A : \mathbb{R}^3 \rightarrow \mathfrak{so}(3)$, which is constant with constant \bar{A} .

The body is assumed to undergo deformations. Its behaviour is governed by a set of equations and constitutive relations. The following is a list of variables and parameters used throughout the paper:

- φ is the deformation of the body;
- $u(x, t) = \varphi(x, t) - x$ is the displacement of the macroscopic material points;
- $F = \nabla\varphi = \mathbb{1} + \nabla u$ is the deformation gradient;
- $F_p = \mathbb{1} + p$ is the plastic distortion which is a non-symmetric tensor with unit determinant, that is, $F_p \in \text{SL}(3)$;
- $F_e = \mathbb{1} + e$ is the elastic distortion which is a non-symmetric tensor;
- $C_p := F_p^T F_p = \mathbb{1} + \varepsilon_p + \dots$ is the positive-definite plastic metric;
- $C_e := F_e^T F_e = \mathbb{1} + \varepsilon_e + \dots$ is the positive-definite elastic strain tensor;

- p is the infinitesimal plastic distortion variable which is a non-symmetric second-order tensor, incapable of sustaining volumetric changes; that is, $p \in \mathfrak{sl}(3)$; the tensor p represents the average plastic slip; p is not gauge-invariant, whereas the rate \dot{p} is;
- $e = \nabla u - p$ is the infinitesimal elastic distortion which is a non-symmetric second-order tensor and is a state-variable;
- $\varepsilon_p = \text{sym } p$ is the symmetric infinitesimal plastic strain tensor, which is also trace free, $\varepsilon_p \in \mathfrak{sl}(3)$; ε_p is not gauge-invariant; the rate $\dot{\varepsilon}_p = \text{sym } \dot{p}$ is gauge-invariant; ε_p is not a state-variable;
- skew p is called plastic rotation or plastic spin and is not a state-variable;
- $\varepsilon_e = \text{sym}(\nabla u - p)$ is the symmetric infinitesimal elastic strain tensor and is a state-variable;
- σ is the Cauchy stress tensor which is a symmetric second-order tensor and is gauge-invariant;
- σ_0 is the initial yield stress for plastic strain and is gauge-invariant;
- σ_y is the current yield stress for plastic strain and is gauge-invariant;
- f is the body force;
- $\text{Curl } p = -\text{Curl } e = \alpha$ is Nye's dislocation density tensor (see (18) for the definition of α), satisfying the so-called Bianchi identities $\text{Div } \alpha = 0$ and is gauge-invariant;
- \mathcal{R} is the Riemann–Christoffel curvature tensor, see (5);
- $\|\mathcal{R}\|^2$ is the Lanczos-type scalar;
- $\text{inc}(\text{sym } p) = \text{inc}(\varepsilon_p) = -\text{inc}(\varepsilon_e)$ is Kröner's second-order incompatibility tensor and is gauge-invariant;
- $\gamma_p = \int_0^t \|\text{sym } \dot{p}\| \, ds$ is the accumulated equivalent plastic strain and is gauge-invariant;
- $\tilde{\gamma}_p = \int_0^t \|\dot{p}\| \, ds$ is the accumulated equivalent plastic distortion and is gauge-invariant.

For isotropic media, the fourth-order isotropic elasticity tensor $\mathbb{C}_{\text{iso}} : \text{Sym}(3) \rightarrow \text{Sym}(3)$ is given by

$$\mathbb{C}_{\text{iso}} X = 2\mu \, \text{dev } \text{sym } X + \kappa \, \text{tr}(X) \mathbb{1} = 2\mu \, \text{sym } X + \lambda \, \text{tr}(X) \mathbb{1} \quad (27)$$

for any second-order tensor X , where μ and λ are the Lamé moduli satisfying

$$\mu > 0 \quad \text{and} \quad 3\lambda + 2\mu > 0, \quad (28)$$

and $\kappa > 0$ is the bulk modulus. These conditions suffice for pointwise ellipticity of the elasticity tensor in the sense that there exists a constant $m_0 > 0$ such that

$$\forall X \in \mathbb{R}^{3 \times 3}: \quad \langle \text{sym } X, \mathbb{C}_{\text{iso}} \text{sym } X \rangle \geq m_0 \|\text{sym } X\|^2. \quad (29)$$

For every $X \in C^1(\Omega, \mathbb{R}^{3 \times 3})$ with rows X_1, X_2, X_3 , we use in this paper the definition of $\text{Curl } X$ in [16, 67]:

$$\text{Curl } X = \begin{pmatrix} \text{curl } X_1 & - & - \\ \text{curl } X_2 & - & - \\ \text{curl } X_3 & - & - \end{pmatrix} \in \mathbb{R}^{3 \times 3}, \quad (30)$$

for which $\text{Curl } \nabla v = 0$ for every $v \in C^2(\Omega, \mathbb{R}^3)$. Note that the definition of $\text{Curl } X$ above is such that $(\text{Curl } X)^T a = \text{curl}(X^T a)$ for every $a \in \mathbb{R}^3$ and this clearly corresponds to the transpose of the Curl of a tensor as defined in [17, 22].

For

$$\bar{A} = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix} \in \mathfrak{so}(3),$$

we consider the operator $\text{axl} : \mathfrak{so}(3) \rightarrow \mathbb{R}^3$ and $\text{anti} : \mathbb{R}^3 \rightarrow \mathfrak{so}(3)$ through

$$\text{axl}(\bar{A}) := (a_1, a_2, a_3)^T, \quad \bar{A} \cdot v = (\text{axl } \bar{A}) \times v, \quad (\text{anti}(v))_{ij} = \varepsilon_{jik} v_k, \quad \forall v \in \mathbb{R}^3, \quad (31)$$

$$(\text{axl } \bar{A})_k = -\frac{1}{2} \sum_{i,j=1}^3 \epsilon_{ijk} \bar{A}_{ij} = \frac{1}{2} \sum_{i,j=1}^3 \epsilon_{kij} \bar{A}_{ji}, \quad (32)$$

$$\bar{A}_{ij} = \sum_{k=1}^3 -\epsilon_{ijk} (\text{axl } \bar{A})_k =: \text{anti}(\text{axl } \bar{A})_{ij}, \quad (33)$$

$$\text{axl}(\text{anti}(v))_k = v_k, \quad (34)$$

where ϵ_{ijk} is the totally antisymmetric third-order Levi-Civita permutation tensor defined by

$$\epsilon_{ijk} := \begin{cases} 1 & \text{if } \{i,j,k\} = \{1,2,3\}, \{2,3,1\} \text{ or } \{3,1,2\}, \\ -1 & \text{if } \{i,j,k\} = \{2,1,3\}, \{1,3,2\} \text{ or } \{3,2,1\}, \\ 0 & \text{if an index is repeated.} \end{cases}$$

Hence, the operators $\text{axl} : \mathfrak{so}(3) \rightarrow \mathbb{R}^3$ and $\text{anti} : \mathbb{R}^3 \rightarrow \mathfrak{so}(3)$ are canonical identifications of $\mathfrak{so}(3)$ and \mathbb{R}^3 . Note that,

$$\begin{aligned} (\text{axl skew } A)_k &= \frac{1}{2} \sum_{i,j=1}^3 \epsilon_{kij} \text{skew}(A)_{ji} = \frac{1}{4} \sum_{i,j=1}^3 \epsilon_{kij} A_{ji} - \frac{1}{4} \sum_{i,j=1}^3 \epsilon_{kij} A_{ji} \\ &= \frac{1}{2} \sum_{i,j=1}^3 \epsilon_{kij} A_{ji} \quad \forall A \in \mathbb{R}^{3 \times 3}. \end{aligned} \quad (35)$$

The following function spaces and norms will also be used later.

$$\begin{aligned} \text{H}(\text{Curl}; \Omega, \mathbb{R}^{3 \times 3}) &:= \left\{ X \in L^2(\Omega, \mathbb{R}^{3 \times 3}) \mid \text{Curl } X \in L^2(\Omega, \mathbb{R}^{3 \times 3}) \right\}, \\ \|X\|_{\text{H}(\text{Curl}; \Omega)}^2 &:= \|X\|_{L^2(\Omega)}^2 + \|\text{Curl } X\|_{L^2(\Omega)}^2, \quad \forall X \in \text{H}(\text{Curl}; \Omega, \mathbb{R}^{3 \times 3}), \\ \text{H}(\text{Curl}; \Omega, \mathbb{E}) &:= \left\{ X : \Omega \rightarrow \mathbb{E} \mid X \in \text{H}(\text{Curl}; \Omega, \mathbb{R}^{3 \times 3}) \right\}, \end{aligned} \quad (36)$$

for $\mathbb{E} := \mathfrak{sl}(3)$ or $\text{Sym}(3) \cap \mathfrak{sl}(3)$.

We also consider the space

$$\text{H}_0(\text{Curl}; \Omega, \Gamma, \mathbb{R}^{3 \times 3}) \quad (37)$$

as the completion in the norm in (36) of the space $\{q \in C^\infty(\Omega, \Gamma, \mathbb{R}^{3 \times 3}) \mid q \times n|_\Gamma = 0\}$. Therefore, this space generalizes the tangential Dirichlet boundary condition

$$q \times n|_\Gamma = 0 \quad (38)$$

to be satisfied by the plastic distortion p or the plastic strain $\varepsilon_p := \text{sym } p$. Whenever, $\Gamma = \partial\Omega$, we simply write $\text{H}_0(\text{Curl}; \Omega, \mathbb{R}^{3 \times 3})$. The space

$$\text{H}_0(\text{Curl}; \Omega, \Gamma, \mathbb{E})$$

is defined as in (36).

The divergence operator Div on second-order tensor-valued functions is also defined row-wise as

$$\text{Div } X = \begin{pmatrix} \text{div } X_1 \\ \text{div } X_2 \\ \text{div } X_3 \end{pmatrix}. \quad (39)$$

Further properties of Kröner's incompatibility tensor inc can be found in the appendix.

3. Discussion of some invariance conditions in plasticity

3.1. Gauge-invariance: invariance under compatible transformations of the reference system

Since the modelling should be invariant with respect to the used coordinate system, we may introduce the *gauge-invariance* condition.

Consider again the multiplicative split $F(x) = F_e(x)F_p(x)$ and perform a compatible change of the reference configuration, i.e., set $x = \psi(\xi)$. Then we have upon transforming to new coordinates

$$F(\psi(\xi)) \nabla_\xi \psi(\xi) = F_e(\psi(\xi)) F_p(\psi(\xi)) \nabla_\xi \psi(\xi). \quad (40)$$

Therefore, we require our new model to be *form-invariant* under

$$\begin{array}{l} F(x) \longrightarrow F(\psi(\xi)) \nabla_\xi \psi(\xi) \quad \forall \psi \in C^\infty(\mathbb{R}^3, \mathbb{R}^3) \\ F_p(x) \longrightarrow F_p(\psi(\xi)) \nabla_\xi \psi(\xi) \quad \text{(Finite Gauge-Invariance)} \end{array} \quad \text{(FGI)}$$

Performing a geometrical linearization, we obtain

$$F(x) = F_e(x)F_p(x) \longrightarrow \nabla u = e(x) + p(x)$$

and the finite gauge-invariance (FGI) translates into direct invariance under

$$\begin{array}{l} \nabla u(x) \longrightarrow \nabla u(\xi) + \nabla \vartheta(\xi) \quad \forall \vartheta \in C^\infty(\mathbb{R}^3, \mathbb{R}^3) \\ p(x) \longrightarrow p(\xi) + \nabla \vartheta(\xi) \quad \text{(Linear Gauge-Invariance)} \end{array} \quad \text{(LGI)}$$

which is also known as *translational gauge-invariance* (see [68–70]).

3.2. Micro-randomness: a novel rotational invariance postulate for polycrystals

Polycrystals can be viewed as random aggregates of single crystals, which at sufficiently large scales can be viewed as isotropic.

Imagine a given initial distribution $F_p(x, 0)$ of grains and subject the polycrystal to a given mechanical loading which alters the plastic state. The result will be recorded in the history $t \rightarrow F_p(x, t)$.

Now consider a randomly rotated initial distribution of grains and plastic distortions via

$$\tilde{F}_p(x, 0) := Q(x)F_p(x, 0) \quad \text{with } Q(x) \in \text{SO}(3). \quad (41)$$

At a sufficiently large scale we are not able to discern this rotational rearrangement and we are led to assume that the new plastic history under the same given loading as before should be

$$t \rightarrow \tilde{F}_p(x, t) := Q(x)F_p(x, t). \quad (42)$$

This is essentially a new invariance requirement to be imposed on our model for the polycrystal. It means that, up to the initially different inhomogeneous rotation of the grains, the response is the same. As rotations are involved, one might take this as a statement of classical isotropy. However, this would be misguided because classical isotropy is concerned with rigidly rotating the whole (polycrystalline) sample, whereas here each individual grain is rotated differently⁹ (see the explanation in Figure 1).

Considering now the geometrically linear setting, we compare the initial infinitesimal plastic distortion $p(x, 0)$ with solution $t \rightarrow p(x, t)$ versus $p(x, 0) + A(x)$ with its time evolution $t \rightarrow \tilde{p}(x, t)$. Our *micro-randomness invariance* condition postulates in the geometrically linear setting that

$$\begin{array}{l} p(x, 0) \rightarrow \tilde{p}(x, 0) = p(x, 0) + A(x) \Rightarrow \\ p(x, t) \rightarrow \tilde{p}(x, t) = p(x, t) + A(x) \quad \forall t > 0 \end{array} \quad \text{(Linear Micro-Random)} \quad \text{(LMR)}$$

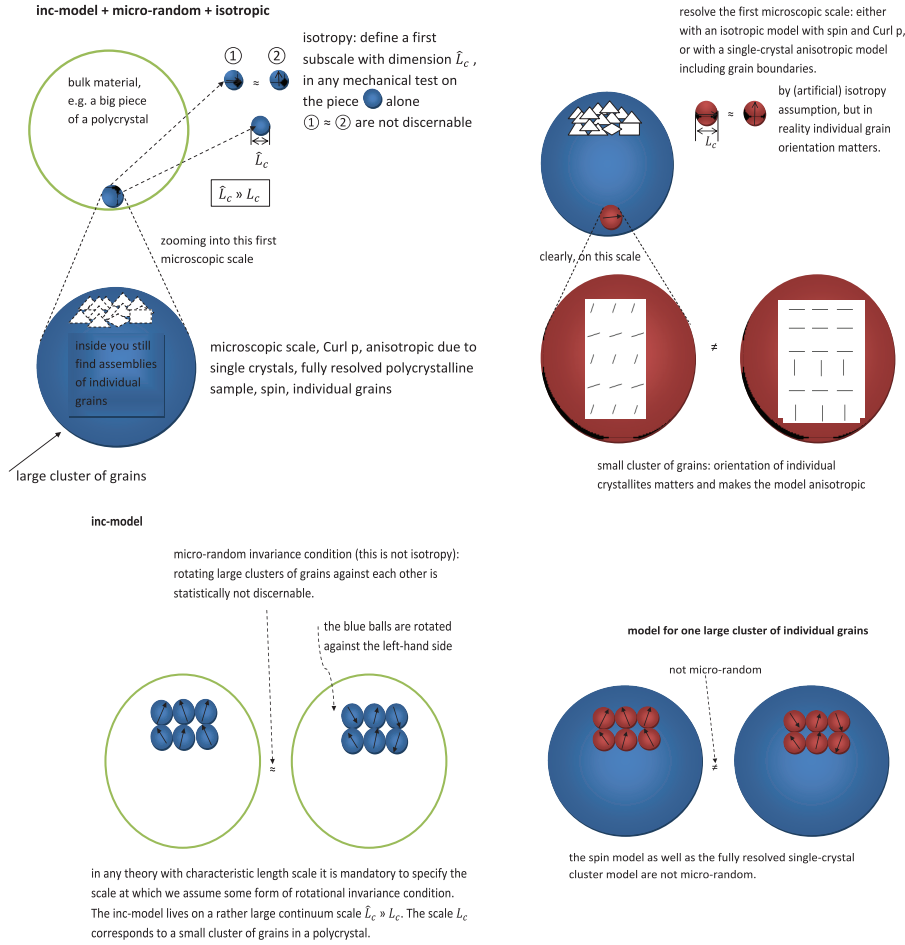


Figure 1. The micro-random model does not resolve a scale smaller than \widehat{L}_c (blue-filled balls). Inside the blue-filled balls, we have crystallites; if we want to model what happens inside there, we can still try to model this with an isotropy assumption. This is our isotropic Curl p -model with spin (see Table 6). In reality however, the orientation of the crystallites matters.

and in the finite deformation setting that

$$\begin{array}{l}
 F_p(x, 0) \rightarrow \widetilde{F}_p(x, 0) = Q(x) F_p(x, 0) \\
 F_p(x, t) \rightarrow \widetilde{F}_p(x, t) = Q(x) F_p(x, t) \quad \forall t > 0
 \end{array}
 \quad \text{(Finite Micro-Random)} \quad . \quad \text{(FMR)}$$

In addition, we are aware of the fact that determining exact initial conditions for the rotations of grains in a polycrystal is practically impossible. Therefore, the influence of considering different initial grain distributions should be minimized in order to obtain a suitable effective model. Our micro-randomness invariance condition ensures that the effect of different initial conditions shows only as an “offset” of an otherwise unique response, as seen above.

Note that

$$\left. \begin{array}{l}
 F(x) = F_e(x) F_p(x) = F_e(x) \underbrace{Q(x)^T Q(x)}_{=1} F_p(x) \\
 \nabla u = e(x) + p(x) = e + \underbrace{A^T(x) + A(x)}_{=0} + p(x)
 \end{array} \right\} \quad Q(x) = \exp(A(x)), \quad (43)$$

thus the invariance condition connected to *micro-randomness* reads in the finite strain case

$$(F, F_e, F_p) \longrightarrow (F, F_e Q^T(x), Q F_p(x)) \quad \forall Q(x) \in \text{SO}(3), \quad (44)$$

Table 3. Invariance conditions for infinitesimal gradient plasticity.

Objectivity/Linearized frame-indifference:	$\begin{cases} \nabla u & \longrightarrow \bar{A} + \nabla u, \\ p & \longrightarrow \bar{A} + p \end{cases}$	$\bar{A} \in \mathfrak{so}(3)$
Linearized gauge-invariance:	$\begin{cases} \nabla u & \longrightarrow \nabla u + \nabla \vartheta, \\ p & \longrightarrow p + \nabla \vartheta \end{cases}$	$\vartheta \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$
Linearized micro-randomness:	$p \longrightarrow p + A(x)$	$A(x) \in \mathfrak{so}(3)$
Isotropy:	$\begin{cases} h : \mathbb{R}^3 \rightarrow \mathbb{R} & \longrightarrow h^\sharp & \text{with } h^\sharp(\xi) := h(Q^T \xi), \\ \phi : \mathbb{R}^3 \rightarrow \mathbb{R}^3 & \longrightarrow \phi^\sharp & \text{with } \phi^\sharp(\xi) := Q \phi(Q^T \xi), \\ S : \mathbb{R}^3 \rightarrow \mathbb{R}^{3 \times 3} & \longrightarrow S^\sharp & \text{with } S^\sharp(\xi) := Q S(Q^T \xi) Q^T \end{cases}$	$Q \in O(3)$

while in the geometrically linear context, we need to require the invariance

$$(\nabla u, e, p) \longrightarrow (\nabla u, e + A^T(x), A(x) + p(x)) \quad \forall A(x) \in \mathfrak{so}(3). \quad (45)$$

3.3. Isotropy in geometrically linear models

Whereas the above invariance conditions can be characterized by additive operators, for classical isotropy we need the group of rotations $Q \in O(3)$. We define isotropy in geometrically linear models to be *form-invariance* under simultaneous change of spatial and referential coordinates by a rigid rotation. In this case, scalar functions $h : \mathbb{R}^3 \rightarrow \mathbb{R}$, vector fields $\phi : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ and second-order tensor fields $S : \mathbb{R}^3 \rightarrow \mathbb{R}^{3 \times 3}$ are transformed as follows:

$$\left. \begin{aligned} h &\longrightarrow h^\sharp && \text{with } h^\sharp(\xi) := h(Q^T \xi), \\ \phi &\longrightarrow \phi^\sharp && \text{with } \phi^\sharp(\xi) := Q \phi(Q^T \xi), \\ S &\longrightarrow S^\sharp && \text{with } S^\sharp(\xi) := Q S(Q^T \xi) Q^T. \end{aligned} \right\} \quad (46)$$

It can be shown (see [72]) that

$$\text{Curl}_\xi [p^\sharp(\xi)] = Q(\text{Curl}_x p(x)) Q^T \quad \text{and} \quad \text{inc}_\xi [\text{sym} p^\sharp(\xi)] = Q \text{inc}_x [\text{sym} p(x)] Q^T. \quad (47)$$

Therefore, both our incompatibility measures are properly isotropic and therefore all our presented models, based on $\text{Curl } p$ or $\text{inc}(\text{sym } p)$, respectively, are fully isotropic.

A summary of the invariance conditions for infinitesimal gradient plasticity is presented in Table 3.

4. Some models of gradient plasticity with Kröner's incompatibility tensor

Before we introduce and analyze our “ideal” model designed from the set of requirements presented in the introduction, we found that it is more interesting to first present those few models we first considered with an emphasis on the difficulties and shortcomings of those models both from the mechanical and mathematical points of view. Let us first make it clear that the approach used to analyze those models as well as our model in Section 4.3 is through a convex analytical framework and variational inequalities developed by Han and Reddy [40] for classical plasticity and quite often used for models of gradient plasticity (see [16, 31, 32, 41, 42]) as well.

4.1. An irrotational model with linear kinematic hardening

In this section, we present a model with linear kinematic hardening and Kröner's incompatibility tensor where the plastic variable is symmetric, i.e. a model with no plastic spin. The goal is to find the displacement field u and the infinitesimal plastic strain ε_p in some suitable function spaces such that the content of Table 4 holds. (A modified version of this model is presented in Table 5.)

Table 4. The model with linear kinematic Prager-type hardening and Kröner's incompatibility tensor. The boundary conditions on ε_p cannot be specified from the structure of the model. The problem with this model is the presence of the norm $\|\varepsilon_p\|^2$ which is not linearized gauge-invariant. A careful analysis of the model in the spirit of Section 4.3 will lead to single out the necessity of an L^2 -control of $\text{Curl } \varepsilon_p$, which is also not a priori controlled in the model. Altogether, well-posedness of the model remains unclear. A modified version of this model is presented in Table 5. This model is micro-random, i.e. invariant with respect to $p \rightarrow p + A(x)$, $A(x) \in \mathfrak{so}(3)$, but not linearized gauge-invariant, i.e. not invariant with respect to $p \rightarrow p + \nabla \vartheta$, $\vartheta \in C^\infty(\mathbb{R}^3, \mathbb{R})$.

Additive split of distortion:	$\nabla u = e + p$
Additive split of strain:	$\text{sym } \nabla u = \varepsilon_e + \varepsilon_p$, $\varepsilon_e := \text{sym } e$ and $\varepsilon_p := \text{sym } p$
Equilibrium:	$\text{Div } \sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e$
Free energy:	$\frac{1}{2} \langle \mathbb{C}_{\text{iso}} \varepsilon_e, \varepsilon_e \rangle + \frac{1}{2} \mu k_1 \ \varepsilon_p\ ^2 + \frac{1}{2} \mu \widehat{L}_c^4 \ \text{inc}(\varepsilon_p)\ ^2$
Yield condition:	$\phi(\Sigma_E) := \ \text{dev } \Sigma_E\ - \sigma_0 \leq 0$
where	$\Sigma_E := \sigma + \Sigma_{\text{kin}} + \Sigma_{\text{inc}}$ with $\Sigma_{\text{kin}} := -\mu k_1 \varepsilon_p$, $\Sigma_{\text{inc}} := -\mu \widehat{L}_c^4 \text{inc}(\text{inc } \varepsilon_p) \in \text{Sym}(3)$
Dissipation inequality:	$\int_{\Omega} \langle \Sigma_E, \dot{\varepsilon}_p \rangle dx \geq 0$
Dissipation function:	$\mathcal{D}(q) := \sigma_0 \ q\ $
Flow law in primal form:	$\Sigma_E \in \partial \mathcal{D}(\dot{\varepsilon}_p)$
Flow law in dual form:	$\dot{\varepsilon}_p = \lambda \frac{\text{dev } \Sigma_E}{\ \text{dev } \Sigma_E\ }$, $\lambda = \ \dot{\varepsilon}_p\ $
KKT conditions:	$\lambda \geq 0$, $\phi(\Sigma_E) \leq 0$, $\lambda \phi(\Sigma_E) = 0$
Boundary conditions for ε_p :	to be specified
Function space for ε_p :	$\varepsilon_p(t, \cdot) \in L^2(\Omega, \text{Sym}(3))$, $\text{inc}(\varepsilon_p) \in L^2(\Omega, \text{Sym}(3))$

4.2. A fully isotropic model with isotropic hardening and plastic spin

The model is described completely in Table 6.

4.3. An irrotational model with isotropic hardening

In this section, we discuss a variant of the previous model with linear kinematic hardening replaced by isotropic hardening. The new model will be invariant under linear referential isotropy (LRIso), linear micro-random (LMR), linear gauge-invariance (LGI), linear elastic objectivity, linear elastic isotropy.

4.3.1. Derivation of the model.

The balance equation. The conventional macroscopic force balance leads to the equation of equilibrium

$$\text{Div } \sigma + f = 0 \quad (48)$$

in which σ is the infinitesimal symmetric Cauchy stress and f is the body force.

Constitutive equations. The constitutive equations are obtained from a free-energy imbalance together with a flow law that characterizes plastic behaviour. The total strain ε is additively decomposed into elastic and plastic components ε_e and ε_p , so that

$$\varepsilon = \varepsilon_e + \varepsilon_p \quad (49)$$

with the plastic strain incapable of sustaining volumetric changes; that is, $\text{tr } \varepsilon_p = 0$.

The strain–displacement relation is given by

$$\varepsilon = \text{sym } \nabla u = \frac{1}{2} (\nabla u + \nabla u^T). \quad (50)$$

Table 5. The model with linear kinematic Prager-type hardening and Kröner's incompatibility tensor. The simple regularization term $\|\text{Curl } \varepsilon_p\|^2$ allows us to justify the boundary conditions on ε_p . The problem with this model is the presence of the norms $\|\varepsilon_p\|^2$ and $\|\text{Curl } \varepsilon_p\|^2$ which are both not *linearized gauge-invariant*. Altogether, well-posedness of this modified model is obtained as in Section 4.3, with the difference that uniqueness of the weak solution is obtained without any additional regularity assumption. This model is micro-random, i.e. invariant with respect to $p \rightarrow p + A(x)$, $A(x) \in \mathfrak{so}(3)$, but not linearized gauge-invariant, i.e. not invariant with respect to $p \rightarrow p + \nabla \vartheta$, $\vartheta \in C^\infty(\mathbb{R}^3, \mathbb{R})$.

Additive split of distortion:	$\nabla u = e + p$
Additive split of strain:	$\text{sym } \nabla u = \varepsilon_e + \varepsilon_p$, $\varepsilon_e := \text{sym } e$ and $\varepsilon_p := \text{sym } p$
Equilibrium:	$\text{Div } \sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e$
Free energy:	$\frac{1}{2} \langle \mathbb{C}_{\text{iso}} \varepsilon_e, \varepsilon_e \rangle + \frac{1}{2} \mu k_1 \ \varepsilon_p\ ^2 + \frac{1}{2} \mu L_c^2 \ \text{Curl } \varepsilon_p\ ^2 + \frac{1}{2} \mu \widehat{L}_c^4 \ \text{inc}(\varepsilon_p)\ ^2$
Yield condition:	$\phi(\Sigma_E) := \ \text{dev } \Sigma_E\ - \sigma_0 \leq 0$ $\Sigma_E := \sigma + \Sigma_{\text{kin}} + \Sigma_{\text{curl}} + \Sigma_{\text{inc}}$, $\Sigma_{\text{kin}} := -\mu k_1 \varepsilon_p$
where	$\Sigma_{\text{curl}} := -\mu L_c^2 \text{sym Curl sym Curl } \varepsilon_p \in \text{Sym}(3)$ $\Sigma_{\text{inc}} := -\mu \widehat{L}_c^4 \text{inc}(\text{inc } \varepsilon_p) \in \text{Sym}(3)$
Dissipation inequality:	$\int_{\Omega} \langle \Sigma_E, \dot{\varepsilon}_p \rangle dx \geq 0$
Dissipation function:	$\mathcal{D}(q) := \sigma_0 \ q\ $
Flow law in primal form:	$\Sigma_E \in \partial \mathcal{D}(\dot{\varepsilon}_p)$
Flow law in dual form:	$\dot{\varepsilon}_p = \lambda \frac{\text{dev } \Sigma_E}{\ \text{dev } \Sigma_E\ }$, $\lambda = \ \dot{\varepsilon}_p\ $
KKT conditions:	$\lambda \geq 0$, $\phi(\Sigma_E) \leq 0$, $\lambda \phi(\Sigma_E) = 0$
Boundary conditions for ε_p :	$\varepsilon_p \times n _{\partial\Omega} = 0$ and $(\text{Curl } \varepsilon_p)^T \times n _{\partial\Omega} = 0$
Function space for ε_p :	$\varepsilon_p(t, \cdot) \in L^2(\Omega, \text{Sym}(3))$, $\text{inc}(\varepsilon_p) \in L^2(\Omega, \text{Sym}(3))$

Table 6. A fully isotropic model with isotropic hardening and plastic spin. The model is fully isotropic because it is form-invariant under the \sharp -transformation defined in (46). The model is also linearized gauge-invariant, i.e. invariant with respect to $p \rightarrow p + \nabla \vartheta$, $\vartheta \in C^\infty(\mathbb{R}^3, \mathbb{R})$, but not micro-random, i.e. not invariant with respect to $p \rightarrow p + A(x)$, $A(x) \in \mathfrak{so}(3)$.

Additive split of distortion:	$\nabla u = e + p$, $\varepsilon_e = \text{sym } e$, $\varepsilon_p = \text{sym } p$
Equilibrium:	$\text{Div } \sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e$
Free energy:	$\frac{1}{2} \langle \mathbb{C}_{\text{iso}} \varepsilon_e, \varepsilon_e \rangle + \frac{1}{2} \mu k_2 \tilde{\gamma}_p ^2 + \frac{1}{2} \mu L_c^2 \ \text{Curl } p\ ^2$
Yield condition:	$\phi(\Sigma_E, g) := \ \text{dev } \Sigma_E\ - (\sigma_0 - g) \leq 0$ where $g := -\mu k_2 \tilde{\gamma}_p$ $\Sigma_E := \sigma + \Sigma_{\text{curl}}$, $\Sigma_{\text{curl}} := -\mu L_c^2 \text{Curl Curl } p$
Dissipation inequality:	$\int_{\Omega} [\langle \Sigma_E, \dot{p} \rangle + g \tilde{\gamma}_p] dx \geq 0$
Dissipation function:	$\mathcal{D}(\dot{\varepsilon}_p, \tilde{\gamma}_p) := \begin{cases} \ \dot{p}\ & \text{if } \ \dot{p}\ \leq \tilde{\gamma}_p, \\ \infty & \text{otherwise} \end{cases}$
Flow law in primal form:	$(\Sigma_E, g) \in \partial \mathcal{D}(\dot{\varepsilon}_p, \tilde{\gamma}_p)$
Flow law in dual form:	$\dot{p} = \lambda \frac{\text{dev } \Sigma_E}{\ \text{dev } \Sigma_E\ }$, $\tilde{\gamma}_p = \lambda = \ \dot{p}\ $
KKT conditions:	$\lambda \geq 0$, $\phi(\Sigma_E, g) \leq 0$, $\lambda \phi(\Sigma_E, g) = 0$
Boundary conditions for p :	$p \times n _{\Gamma} = 0$, $\text{Curl } p \times n _{\partial\Omega \setminus \Gamma} = 0$

Free-energy density. In this model the free-energy density is considered in the additively separated form

$$W(u, \varepsilon_p, \text{inc } \varepsilon_p, \gamma_p) := \underbrace{W_e(\varepsilon_e)}_{\text{elastic energy}} + \underbrace{W_{\text{inc}}(\text{inc } \varepsilon_p)}_{\text{mesoscopic incompatibility}} + \underbrace{W_{\text{iso}}(\gamma_p)}_{\text{isotropic hardening energy (SSD-related)}}, \quad (51)$$

where

$$\left. \begin{aligned} W_c(\varepsilon_e) &:= \frac{1}{2} \langle \varepsilon_e, \mathbb{C}_{\text{iso}} \varepsilon_e \rangle = \mu \|\text{sym } \nabla u - \varepsilon_p\|^2 + \frac{1}{2} \lambda \text{tr}[\nabla u - \varepsilon_p]^2, \\ W_{\text{inc}}(\text{inc } \varepsilon_p) &:= \frac{1}{2} \mu \widehat{L}_c^4 \|\text{inc } \varepsilon_p\|^2 = \frac{1}{2} \mu \widehat{L}_c^4 \|\text{Curl}[(\text{Curl } \varepsilon_p)^T]\|^2, \\ W_{\text{iso}}(\gamma_p) &:= \frac{1}{2} \mu k_2 |\gamma_p|^2, \end{aligned} \right\} \quad (52)$$

and λ, μ are the Lamé moduli with $\mu > 0$ and $3\lambda + 2\mu > 0, \widehat{L}_c \geq 0$ is an energetic length scale and $k_2 > 0$ is a positive non-dimensional isotropic hardening constant, γ_p is the isotropic hardening variable (the accumulated equivalent plastic strain).

From the local free-energy imbalance

$$\begin{aligned} \frac{d}{dt} W \leq \langle \sigma, \nabla u_t \rangle = \langle \sigma, \dot{\varepsilon} \rangle &\Leftrightarrow \frac{d}{dt} W - \langle \sigma, \dot{\varepsilon} \rangle - \langle \sigma, \dot{\varepsilon}_p \rangle \leq 0 \\ &\Leftrightarrow \frac{d}{dt} W(u, \varepsilon_p, D^2 \varepsilon_p, \gamma_p) \leq 0 \quad \text{for } u \text{ fixed} \end{aligned}$$

where the second equivalence is obtained using arguments from thermodynamics which give the elasticity relation

$$\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e = 2\mu (\text{sym } \nabla u - \varepsilon_p) + \lambda \text{tr}(\text{sym } \nabla u - \varepsilon_p) \mathbb{1}. \quad (53)$$

Therefore, we obtain

$$\langle \sigma, \dot{\varepsilon}_p \rangle - \mu \widehat{L}_c^4 \langle \text{inc } \varepsilon_p, \text{inc } \dot{\varepsilon}_p \rangle - \mu k_2 \gamma_p \dot{\gamma}_p \geq 0. \quad (54)$$

Now, integrating (54), we arrive at

$$\begin{aligned} 0 &\leq \int_{\Omega} \left[\langle \sigma, \dot{\varepsilon}_p \rangle - \underbrace{\mu \widehat{L}_c^4 \langle \text{inc}(\text{inc } \varepsilon_p), \dot{\varepsilon}_p \rangle}_{\in \text{Sym}(3)} - \mu k_2 \gamma_p \dot{\gamma}_p - \sum_{i=1}^3 \text{div} \left(\mu \widehat{L}_c^4 \dot{\varepsilon}_{pi} \times [\text{Curl inc } \varepsilon_p]_i^T \right) \right. \\ &\quad \left. - \sum_{i=1}^3 \text{div} \left(\mu \widehat{L}_c^4 [\text{Curl } \dot{\varepsilon}_p]_i^T \times [\text{inc } \varepsilon_p]_i \right) \right] dx \\ &= \int_{\Omega} \left[\langle \sigma - \mu \widehat{L}_c^4 \text{inc}(\text{inc } \varepsilon_p), \dot{\varepsilon}_p \rangle - \mu k_2 \gamma_p \dot{\gamma}_p \right] dx \\ &\quad - \sum_{i=1}^3 \mu \widehat{L}_c^4 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times [\text{Curl inc } \varepsilon_p]_i^T, n \rangle dS - \sum_{i=1}^3 \mu \widehat{L}_c^4 \int_{\partial\Omega} \langle [\text{Curl } \dot{\varepsilon}_p]_i^T \times [\text{inc } \varepsilon_p]_i, n \rangle dS. \end{aligned} \quad (55)$$

In order to obtain a global reduced dissipation inequality one needs to choose suitable boundary conditions for which the following two equations are satisfied

$$\sum_{i=1}^3 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, [\text{Curl inc } \varepsilon_p]_i^T \rangle dS = 0. \quad (56)$$

$$\sum_{i=1}^3 \int_{\partial\Omega} \langle [\text{Curl } \dot{\varepsilon}_p]_i^T \times n, [\text{inc } \varepsilon_p]_i \rangle dS = 0. \quad (57)$$

The simplest lower order boundary conditions to satisfy (56) and (57) are

$$\varepsilon_p \times n|_{\partial\Omega} = 0 \quad \text{and} \quad [\text{Curl } \varepsilon_p]^T \times n|_{\partial\Omega} = 0. \quad (58)$$

Other possible boundary conditions to satisfy the equations (56) and (57) are given in Table 7.

Table 7. Possible boundary conditions for (56) and (57) to be satisfied.

boundary conditions for (56)	boundary conditions for (57)
$[\text{Curl inc } \varepsilon_p]^T \times n _{\partial\Omega} = 0$	$(\text{inc } \varepsilon_p) \times n _{\partial\Omega} = 0$
$\varepsilon_p \times n _{\Gamma} = 0$ and $[\text{Curl inc } \varepsilon_p]^T \times n _{\partial\Omega \setminus \Gamma} = 0$	$[\text{Curl } \varepsilon_p]^T \times n _{\Gamma} = 0$ and $\text{inc } \varepsilon_p \times n _{\partial\Omega \setminus \Gamma} = 0$.

Table 8. The irrotational model with isotropic hardening and Kröner's incompatibility tensor. The terms in the free-energy density are not enough to guarantee the minimum regularity required, i.e. $\varepsilon_p \in \text{H}(\text{Curl})$ and $(\text{Curl } \varepsilon_p)^T \in \text{H}(\text{Curl})$, in order to justify mathematically the boundary conditions $\varepsilon_p \times n|_{\partial\Omega} = 0$ and $(\text{Curl } \varepsilon_p)^T \times n|_{\partial\Omega} = 0$.

Additive split of strain:	$\text{sym } \nabla u = \varepsilon_e + \varepsilon_p$
Equilibrium:	$\text{Div } \sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e$
Free energy:	$\frac{1}{2} \langle \mathbb{C}_{\text{iso}} \varepsilon_e, \varepsilon_e \rangle + \frac{1}{2} \mu k_2 \gamma_p ^2 + \frac{1}{2} \mu \widehat{L}_c^4 \ \text{inc } \varepsilon_p\ ^2$
Yield condition:	$\phi(\Sigma_E, g) := \ \text{dev } \Sigma_E\ - (\sigma_0 - g) \leq 0$ where $g := -\mu k_2 \gamma_p$ $\Sigma_E := \sigma + \Sigma_{\text{inc}},$ $\Sigma_{\text{inc}} := -\mu \widehat{L}_c^4 \text{inc inc } \varepsilon_p = \text{Curl} \left([\text{Curl Curl} [(\text{Curl } \varepsilon_p)^T]]^T \right)$
Dissipation inequality:	$\int_{\Omega} [(\Sigma_E, \dot{\varepsilon}_p) + g \dot{\gamma}_p] dx \geq 0$
Dissipation function:	$\mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p) := \begin{cases} \sigma_0 \ \dot{\varepsilon}_p\ & \text{if } \ \dot{\varepsilon}_p\ \leq \dot{\gamma}_p, \\ \infty & \text{otherwise} \end{cases}$
Flow law in primal form:	$(\Sigma_E, g) \in \partial \mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p)$
Flow law in dual form:	$\dot{\varepsilon}_p = \lambda \frac{\text{dev } \Sigma_E}{\ \text{dev } \Sigma_E\ }, \quad \dot{\gamma}_p = \lambda = \ \dot{\varepsilon}_p\ $
KKT conditions:	$\lambda \geq 0, \quad \phi(\Sigma_E, g) \leq 0, \quad \lambda \phi(\Sigma_E, g) = 0$
Boundary conditions for ε_p :	$\varepsilon_p \times n _{\partial\Omega} = 0, \quad (\text{Curl } \varepsilon_p)^T \times n _{\partial\Omega} = 0$

However, these boundary conditions cannot be mathematically justified from the free-energy density W considered so far: both terms in (56) and (57) are not automatically well-defined as boundary traces. In fact, one needs to show that $\varepsilon_p \in \text{H}(\text{Curl})$ and $(\text{Curl } \varepsilon_p)^T \in \text{H}(\text{Curl})$. This information is missing from the energy. We only know that $\varepsilon_p \in L^2$ (due to isotropic hardening) and $\text{inc } \varepsilon_p = \text{Curl}[(\text{Curl } \varepsilon_p)^T] \in L^2$. The missing piece of information to proceed is $\text{Curl } \varepsilon_p \in L^2$.

Thus, one needs to modify the model by adding a new regularizing term in the free-energy density W , which is physically meaningful in the sense that it does satisfy some invariance properties. The unmodified model is summarized in Table 8.

We will consider the additional term

$$W_{\text{curl}}(\text{Curl } p) := \frac{1}{2} \mu L_c^2 \|\text{dev sym Curl } \varepsilon_p\|^2, \quad (59)$$

which is motivated in the following section.

4.3.2. Conformal gauge-invariance: the regularization term $\text{dev sym Curl } \varepsilon_p$.

We show subsequently that the model with the regularizing term $\text{dev sym Curl } \varepsilon_p$ allows for a mathematical existence proof. However, what about the invariance conditions, notably gauge-invariance?

It is easy to see that

$$p \rightarrow \text{dev sym Curl } \varepsilon_p = \text{dev sym Curl sym } p$$

is micro-random whereas it is not linear gauge-invariant, i.e.

$$\begin{aligned} p &\rightarrow p + \nabla \vartheta \\ \text{dev sym Curl sym}(\nabla \vartheta + p) &\neq \text{dev sym Curl sym } p \quad \forall \vartheta \in C^1(\Omega, \mathbb{R}^3). \end{aligned} \quad (60)$$

Let us now determine those mappings $\vartheta : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ that are still “allowed” for gauge-invariance, in the sense that

$$\text{dev sym Curl sym}(\nabla \vartheta + p) = \text{dev sym Curl sym } p.$$

Automatically, these mappings satisfy the identity $\text{inc}(\text{sym } \nabla \vartheta) = 0$. Moreover, by linearity we should have

$$\text{dev sym Curl sym } \nabla \vartheta = 0. \quad (61)$$

However, because $\text{tr}(\text{Curl } S) = 0$ for all smooth symmetric tensor fields $S \in \text{Sym}(3)$ (see (109) in the appendix), the latter is equivalent to

$$\text{sym Curl sym } \nabla \vartheta = 0.$$

This implies that for some non-constant skew-symmetric tensor field $A : \Omega \rightarrow \mathfrak{so}(3)$ we have

$$\text{Curl sym } \nabla \vartheta(x) = A(x) \quad \Leftrightarrow \quad (\text{Curl sym } \nabla \vartheta)^T = -A(x). \quad (62)$$

Taking the Curl on both sides leads to

$$\text{Curl}[(\text{Curl sym } \nabla \vartheta)^T] = -\text{Curl } A(x) \quad \Leftrightarrow \quad 0 = \text{inc}(\text{sym } \nabla \vartheta) = -\text{Curl } A(x). \quad (63)$$

Thus, $A(x) = \bar{A}$ is a constant skew-symmetric matrix, according to an observation in [72]. Reinserting into (62), we must have

$$\text{Curl sym } \nabla \vartheta(x) = \bar{A}. \quad (64)$$

We observe that (see [73])

$$\text{Curl}(\zeta(x_1, x_2, x_3) \cdot \mathbb{1}) = \begin{pmatrix} 0 & -\zeta_{3,2} & \zeta_{2,3} \\ \zeta_{3,1} & 0 & -\zeta_{1,3} \\ -\zeta_{2,1} & \zeta_{1,2} & 0 \end{pmatrix} \quad \zeta : \mathbb{R}^3 \rightarrow \mathbb{R}$$

and with $\zeta(x_1, x_2, x_3) = ax_1 + bx_2 + cx_3$, we obtain

$$\text{Curl}((ax_1 + bx_2 + cx_3) \cdot \mathbb{1}) = \begin{pmatrix} 0 & -c & b \\ c & 0 & -a \\ -b & a & 0 \end{pmatrix}.$$

Hence, a solution to (64) can be obtained in the format

$$\text{sym } \nabla \vartheta(x_1, x_2, x_3) = \zeta(x_1, x_2, x_3) \cdot \mathbb{1}. \quad (65)$$

On taking again the deviatoric part of the latter we arrive at

$$\text{dev sym } \nabla \vartheta(x_1, x_2, x_3) = 0. \quad (66)$$

This is equivalent to

$$\nabla \vartheta(x) = \zeta(x_1, x_2, x_3) \cdot \mathbb{1} + A(x_1, x_2, x_3) \quad \text{with } A : \mathbb{R}^3 \rightarrow \mathfrak{so}(3). \quad (67)$$

The solution to (66) can be given in closed form. In fact, taking Curl on both sides of (67), together with the fact that $\text{Curl}(\zeta(x_1, x_2, x_3) \cdot \mathbb{1}) \in \mathfrak{so}(3)$, one obtains $A(x_1, x_2, x_3) = \bar{A} \in \mathfrak{so}(3)$ constant skew-symmetric matrix. In addition, using the operators axl and anti defined in (31), a general solution to (66) is obtained in the form

$$\phi_c(x) := \frac{1}{2} \left(2 \langle \text{axl}(\widehat{W}), x \rangle x - \text{axl}(\widehat{W}) \|x\|^2 \right) + [\widehat{\zeta} \cdot \mathbb{1} + \widehat{A}]x + \widehat{\eta}, \quad (68)$$

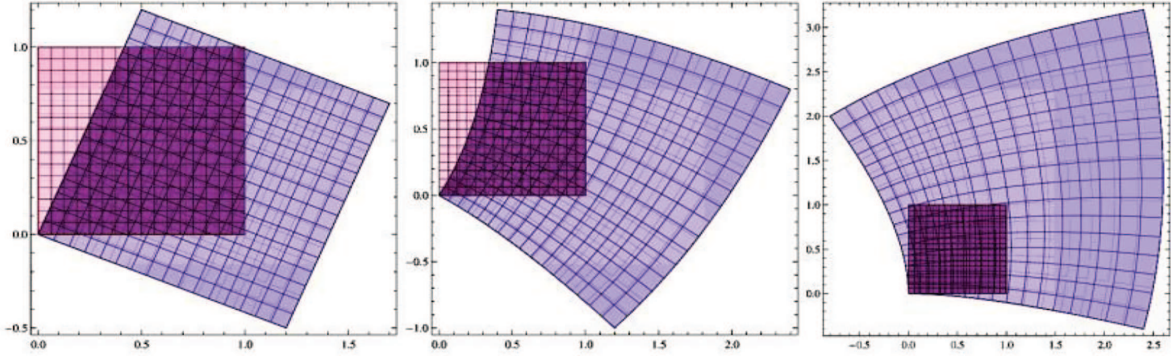


Figure 2. Infinitesimal conformal mappings $\phi_c : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ that locally leave shapes invariant: a prototype elastic deformation in the sense that the corresponding stress deviator $\text{dev } \sigma(\nabla \phi_c) = 0$. Shown is the coarse grid deformation. Reproduced with permission from [74].

where $\widehat{A}, \widehat{W} \in \mathfrak{so}(3)$ are arbitrary constant skew-symmetric matrices and $\widehat{\zeta}, \widehat{\eta} \in \mathbb{R}^3$ are arbitrary constant vectors.

The mappings in (68) are called *infinitesimal conformal mappings* ϕ_c (see [74]). The mappings $x \rightarrow \phi_c(x)$ locally preserve the shape of infinitesimal cubes but are globally inhomogeneous.

If we consider $x \rightarrow \phi_c(x)$ as elastic displacement, then, according to the von Mises J_2 -criterion, these mappings alone never lead to plasticity because

$$\text{dev } \sigma = \text{dev}(2 \mu \text{sym } \nabla \phi_c + \lambda \text{tr}(\nabla \phi_c \cdot \mathbb{1})) = 2 \mu \text{dev sym } \nabla \phi_c = 0.$$

Gathering our findings, we have obtained that the regularization term (59) is invariant with respect to the infinitesimal conformal group and infinitesimal conformal mappings ϕ_c do not induce irreversible processes.

There is still another solution to

$$\text{sym Curl sym } \nabla \vartheta = 0. \tag{69}$$

Clearly, (69) will be satisfied also if already

$$\text{Curl sym } \nabla \vartheta = 0,$$

which, in turn, is satisfied for $\text{sym } \nabla \vartheta = \nabla v \in \text{Sym}(3)$, with $v : \mathbb{R}^3 \rightarrow \mathbb{R}^3$. Such a vector can be taken as $v = \nabla h(x_1, x_2, x_3)$ with any scalar function $h : \mathbb{R}^3 \rightarrow \mathbb{R}$. Then, (69) is satisfied. Thus, another solution to (69) is given by

$$\vartheta(x_1, x_2, x_3) = \nabla h(x_1, x_2, x_3), \quad h : \mathbb{R}^3 \rightarrow \mathbb{R}.$$

Altogether, solutions to (69) are represented by

$$\vartheta(x) = \underbrace{\phi_c(x)}_{\text{“conformal”}} + \underbrace{\nabla h}_{\text{“potential”}}$$

as the new invariance group. We collect our finding in the following theorem.

Theorem 4.1 (Nullspace of dev sym Curl sym Grad). *The nullspace of the operator dev sym Curl sym Grad is given by*

$$\vartheta(x) = \frac{1}{2} \left(2 \langle \text{axl}(\widehat{W}), x \rangle x - \text{axl}(\widehat{W}) \|x\|^2 \right) + [\widehat{\zeta} \cdot \mathbb{1} + \widehat{A}]x + \widehat{\eta} + \nabla h(x),$$

where $\widehat{A}, \widehat{W} \in \mathfrak{so}(3)$ are arbitrary constant skew-symmetric matrices, $\widehat{\zeta}, \widehat{\eta} \in \mathbb{R}^3$ are arbitrary constant vectors and $h : \mathbb{R}^3 \rightarrow \mathbb{R}$ is any scalar function.

It is remarkable, that the seemingly similar regularization term $\|\text{Curl sym } p\|^2 = \|\text{Curl } \varepsilon_p\|^2$ only allows for invariance under “potential” mappings $\vartheta = \nabla h$.

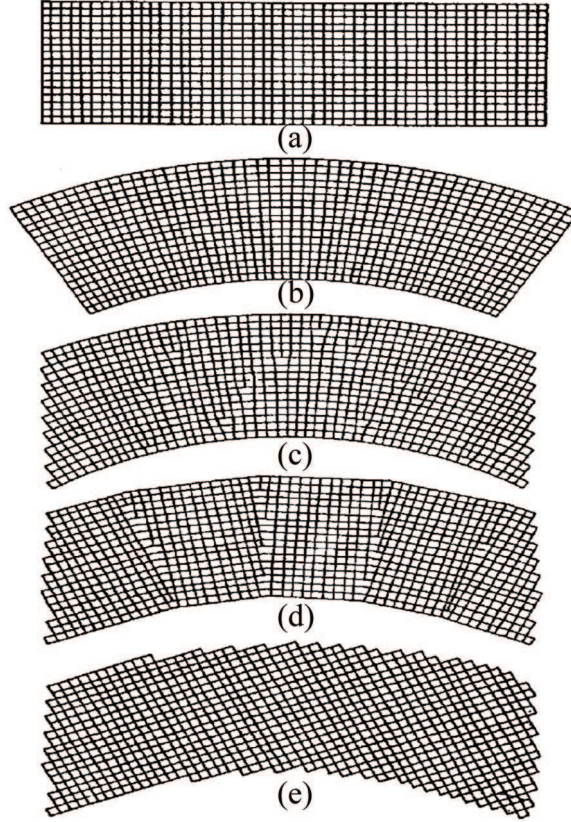


Figure 3. Five states of a single crystal: (a) unstrained; (b) elastically bent; (c) plastically bent; (d) polygonized; (e) recrystallized. For the polygonized crystal, we observe large structures that are rotated against each other with a “zone” separating those blocks. Using plainly $\text{Curl } p$ as the underlying defect measure would energetically penalize these configurations. Therefore, it seems appropriate to use $\text{inc}(\text{sym } p)$ as a “weaker” defect measure which would allow for low-energy configurations such as that in (d). Reproduced with permission from [75].

In order to be able to describe polygonization (see Figure 3(d)), the plasticity model should energetically favour configurations in which there are blocks of many homogeneous rotations.

In this respect, the new term $\frac{1}{2} \mu L_c^2 \|\text{dev sym Curl sym } p\|^2 = \frac{1}{2} \mu L_c^2 \|\text{sym Curl sym } p\|^2$ energetically favours those configurations, which locally only rotate. The generated natural second-order backstress will be of the type

$$\Sigma_{\text{curl}} = \mu L_c^2 \text{sym Curl}(\text{sym Curl } \varepsilon_p).$$

Now, looking at the invariance of the energy for which $\text{sym Curl}(\text{sym } \nabla \vartheta) = 0$ versus the invariance of the backstress in the strong formulation for which $\text{sym Curl}(\text{sym Curl}(\text{sym } \nabla \vartheta)) = 0$, it is clear that the invariance of the energy implies the invariance of backstress, but not vice versa.

Remark 4.1. Note that the mapping $p \rightarrow \text{dev sym Curl sym } p = \text{sym Curl } \varepsilon_p$ does not have any geometric meaning connected to the incompatibility of the plastic distortion p like $\text{Curl } p$ or connected to the incompatibility of the plastic strain tensor $\varepsilon_p = \text{sym } p$ like $\text{inc}(\text{sym } p)$. The simpler term $\text{Curl sym } p$ has been used by Gurtin and Anand [17] as the only energetic contribution in their irrotational gradient plasticity model.

4.3.3. Derivation of the modified model.

Now with the additional term $W_{\text{curl}}(\text{Curl } p) := \frac{1}{2} \mu L_c^2 \|\text{dev sym Curl } \varepsilon_p\|^2 = \frac{1}{2} \mu L_c^2 \|\text{sym Curl } \varepsilon_p\|^2$ in the

free-energy density W , if we repeat the derivation above starting from the free-energy imbalance, we obtain

$$0 \leq \int_{\Omega} \left[\langle \sigma - \mu L_c^2 \operatorname{sym} \operatorname{Curl}(\operatorname{sym} \operatorname{Curl} \varepsilon_p) - \mu \widehat{L}_c^4 \operatorname{inc}(\operatorname{inc} \varepsilon_p), \dot{\varepsilon}_p \rangle - \mu k_2 \gamma_p \dot{\gamma}_p \right] dx \quad (70)$$

$$\begin{aligned} & - \sum_{i=1}^3 \mu L_c^2 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, (\operatorname{sym} \operatorname{Curl} \varepsilon_p)_i \rangle dS - \sum_{i=1}^3 \mu \widehat{L}_c^4 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, [\operatorname{Curl} \operatorname{inc} \varepsilon_p]_i^T \rangle dS \\ & - \sum_{i=1}^3 \mu \widehat{L}_c^4 \int_{\partial\Omega} \langle [\operatorname{Curl} \dot{\varepsilon}_p]_i^T \times n, [\operatorname{inc} \varepsilon_p]_i \rangle dS \\ = & \int_{\Omega} \left[\langle \Sigma_E, \dot{\varepsilon}_p \rangle + g \dot{\gamma}_p \right] dx - \sum_{i=1}^3 \mu L_c^2 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, (\operatorname{sym} \operatorname{Curl} \varepsilon_p)_i \rangle dS \\ & - \sum_{i=1}^3 \mu \widehat{L}_c^4 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, [\operatorname{Curl} \operatorname{inc} \varepsilon_p]_i^T \rangle dS - \sum_{i=1}^3 \mu \widehat{L}_c^4 \int_{\partial\Omega} \langle [\operatorname{Curl} \dot{\varepsilon}_p]_i^T \times n, [\operatorname{inc} \varepsilon_p]_i \rangle dS \end{aligned} \quad (71)$$

where

$$\begin{aligned} \Sigma_E & := \sigma + \Sigma_{\operatorname{curl}} + \Sigma_{\operatorname{inc}}, & g & = -\mu k_2 \gamma_p, \\ \Sigma_{\operatorname{curl}} & := -\mu L_c^2 \operatorname{sym} \operatorname{Curl}(\operatorname{sym} \operatorname{Curl} \varepsilon_p), & & \text{(second-order non-local backstress)} \\ \Sigma_{\operatorname{inc}} & := -\mu \widehat{L}_c^4 \operatorname{inc}(\operatorname{inc} \varepsilon_p) \\ & = -\mu \widehat{L}_c^4 \operatorname{Curl} \left(\left[\operatorname{Curl} \operatorname{Curl} [\operatorname{Curl} \varepsilon_p]^T \right]^T \right) & & \text{(fourth-order non-local backstress)}. \end{aligned}$$

Now assuming again the simplest lower order boundary conditions

$$\varepsilon_p \times n|_{\partial\Omega} = 0 \quad \text{and} \quad [\operatorname{Curl} \varepsilon_p]^T \times n|_{\partial\Omega} = 0, \quad (72)$$

which will be clearly defined as Sobolev traces through a choice of a suitable function space for the plastic strain variable ε_p , will guarantee the insulation-type conditions

$$\sum_{i=1}^3 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, (\operatorname{sym} \operatorname{Curl} \varepsilon_p)_i \rangle dS = 0, \quad (73)$$

$$\sum_{i=1}^3 \int_{\partial\Omega} \langle \dot{\varepsilon}_{pi} \times n, [\operatorname{Curl} \operatorname{inc} \varepsilon_p]_i^T \rangle dS = 0, \quad (74)$$

$$\sum_{i=1}^3 \int_{\partial\Omega} \langle [\operatorname{Curl} \dot{\varepsilon}_p]_i^T \times n, [\operatorname{inc} \varepsilon_p]_i \rangle dS = 0, \quad (75)$$

from which we obtain the global reduced dissipation inequality

$$\int_{\Omega} \left[\langle \Sigma_E, \dot{\varepsilon}_p \rangle + g \dot{\gamma}_p \right] dx \geq 0. \quad (76)$$

The flow law. We consider the set of admissible (elastic) generalized stresses

$$\mathcal{E} := \{(\Sigma_E, g) \mid \|\operatorname{dev} \Sigma_E\| - (\sigma_0 - g) \leq 0, \quad g \leq 0\}, \quad (77)$$

whose interior $\operatorname{Int}(\mathcal{E})$ is the elastic domain while its boundary $\partial\mathcal{E}$ is the yield surface. The constant σ_0 is the initial yield stress of the material. The flow law in its primal form reads as follows:

$$(\Sigma_E, g) \in \partial\mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p) \quad (78)$$

where

$$\begin{aligned} \mathcal{D}(q, \beta) &:= \sup\{\langle \Sigma_E, q \rangle + g\beta \mid (\Sigma_E, g) \in \mathcal{E}\} \\ &= \sup\{\langle \Sigma_E, q \rangle + g\beta \mid \|\Sigma_E\| \leq \sigma_0 - g, \quad g \leq 0\} \\ &= \begin{cases} \sigma_0 \|q\| & \text{if } \|q\| \leq \beta, \\ \infty & \text{otherwise.} \end{cases} \end{aligned} \quad (79)$$

Here, $\partial\mathcal{D}(\dot{\Gamma}_p)$ denotes the subdifferential of the function \mathcal{D} at $\dot{\Gamma}_p$. That is,

$$(\Sigma_E, g) \in \partial\mathcal{D}(\dot{\epsilon}_p, \dot{\gamma}_p) \Leftrightarrow \langle \Sigma_E, q - \dot{\epsilon}_p \rangle + g(\beta - \dot{\gamma}_p) \leq \mathcal{D}(q, \beta) - \mathcal{D}(\dot{\epsilon}_p, \dot{\gamma}_p) \quad \forall (q, \beta). \quad (80)$$

Now using convex analysis, we obtain

$$(\Sigma_E, g) \in \partial\mathcal{D}(\dot{\epsilon}_p, \dot{\gamma}_p) \Leftrightarrow (\dot{\epsilon}_p, \dot{\gamma}_p) \in \partial I_{\mathcal{E}}(\Sigma_E, g) = N_{\mathcal{E}}(\Sigma_E, g), \quad (81)$$

where $I_{\mathcal{E}}$ is the indicator function of the set \mathcal{E} of admissible generalized stresses and $N_{\mathcal{E}}(\Sigma_E, g)$ is the normal cone of the set \mathcal{E} at (Σ_E, g) .

The condition (81)₂ is called the *dual form of the flow law*, which in the case of smoothness of the yield surface $\partial\mathcal{E}$ at (Σ_E, g) gives for some scalar parameter $\lambda \geq 0$

$$\dot{\epsilon}_p = \lambda \frac{\text{dev } \Sigma_E}{\|\text{dev } \Sigma_E\|} \quad \text{and} \quad \dot{\gamma}_p = \lambda = \|\dot{\epsilon}_p\| \quad (82)$$

together with the Karush–Kuhn–Tucker (KKT) complementary conditions:

$$\lambda \geq 0, \quad \phi(\Sigma_E, g) \leq 0 \quad \text{and} \quad \lambda \phi(\Sigma_E, g) = 0.$$

Note that with this choice, the global dissipation inequality (76) is satisfied.

4.3.4. Mathematical strong formulation of the model,

Taking into account the free-energy density W in (51) together with the additional term in (59) and the constraint $\|q\| \leq \beta$ in the definition of the dissipation function \mathcal{D} in (79), the model is strongly formulated as follows. Find:

- (i) the displacement $u \in \mathbf{H}^1(0, T; \mathbf{H}_0^1(\Omega, \Gamma, \mathbb{R}^3))$;
- (ii) the infinitesimal plastic strain $\varepsilon_p \in \mathbf{H}^1(0, T; L^2(\Omega, \mathfrak{sl}(3) \cap \text{Sym}(3)))$ with

$$\begin{aligned} \text{sym Curl } \varepsilon_p &\in \mathbf{H}^1(0, T; L^2(\Omega, \text{Sym}(3) \cap \mathfrak{sl}(3))); \\ \text{inc } \varepsilon_p &= \text{Curl}[(\text{Curl } \varepsilon_p)^T] \in \mathbf{H}^1(0, T; L^2(\Omega, \mathbb{R}^{3 \times 3})); \\ \text{inc inc } \varepsilon_p &= \text{Curl}\left([\text{Curl Curl}[(\text{Curl } \varepsilon_p)^T]]^T\right) \in \mathbf{H}^1(0, T; L^2(\Omega, \mathbb{R}^{3 \times 3})); \end{aligned}$$

- (iii) the internal isotropic hardening variable $\gamma_p \in \mathbf{H}^1(0, T; L^2(\Omega))$;

such that the content of Table 9 holds.

4.3.5. Weak formulation of the model.

To obtain the weak formulation of the model, we consider the equilibrium in its weak formulation. That is, for every $v \in \mathbf{H}_0^1(\Omega, \mathbb{R}^3)$ we have

$$\int_{\Omega} \langle \mathbb{C}_{\text{iso}}(\text{sym } \nabla u - \varepsilon_p), \text{sym}(\nabla v - \nabla \dot{u}) \rangle dx = \int_{\Omega} f(v - \dot{u}) dx. \quad (83)$$

On the other hand, for every $q \in C^\infty(\overline{\Omega}, \mathfrak{sl}(3) \cap \text{Sym}(3))$ such that

$$q \times n|_{\partial\Omega} = 0 \quad \text{and} \quad (\text{Curl } q)^T \times n|_{\partial\Omega} = 0$$

Table 9. The new regularized irrotational model with isotropic hardening and Kröner's incompatibility tensor. Also in this case, the boundary condition on ε_p necessitates at least $\varepsilon_p, (\text{Curl } \varepsilon_p)^T \in H(\text{Curl}; \Omega, \mathbb{R}^{3 \times 3})$. The model is micro-random, i.e. invariant with respect to $p \rightarrow p + A(x)$, $A(x) \in \mathfrak{so}(3)$ and invariant under infinitesimal conformal mappings $p \rightarrow p + \nabla \phi_c$ with $\text{dev sym } \nabla \phi_c = 0$.

Additive split of strain:	$\text{sym } \nabla u = \varepsilon_e + \varepsilon_p$
Equilibrium:	$\text{Div } \sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e$
Free energy:	$\frac{1}{2} \langle \mathbb{C}_{\text{iso}} \varepsilon_e, \varepsilon_e \rangle + \frac{1}{2} \mu k_2 \gamma_p ^2 + \frac{1}{2} \mu L_c^2 \ \text{sym Curl } \varepsilon_p\ ^2 + \frac{1}{2} \mu \widehat{L}_c^4 \ \text{inc } \varepsilon_p\ ^2$
Yield condition:	$\phi(\Sigma_E, g) := \ \text{dev } \Sigma_E\ ^2 - (\sigma_0 - g) \leq 0$ where $g := -\mu k_2 \gamma_p$ $\Sigma_E := \sigma + \Sigma_{\text{curl}} + \Sigma_{\text{inc}},$ $\Sigma_{\text{curl}} := -\mu L_c^2 \text{sym Curl}(\text{sym Curl } \varepsilon_p)$ $\Sigma_{\text{inc}} := -\mu \widehat{L}_c^4 \text{inc inc } \varepsilon_p = \text{Curl}[\text{Curl Curl}[\text{Curl } \varepsilon_p]^T]^T$
Dissipation inequality:	$\int_{\Omega} [(\Sigma_E, \dot{\varepsilon}_p) + g \dot{\gamma}_p] dx \geq 0$
Dissipation function:	$\mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p) := \begin{cases} \sigma_0 \ \dot{\varepsilon}_p\ & \text{if } \ \dot{\varepsilon}_p\ \leq \dot{\gamma}_p, \\ \infty & \text{otherwise} \end{cases}$
Flow law in primal form:	$(\Sigma_E, g) \in \partial \mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p)$
Flow law in dual form:	$\dot{\varepsilon}_p = \lambda \frac{\text{dev } \Sigma_E}{\ \text{dev } \Sigma_E\ }, \quad \dot{\gamma}_p = \lambda = \ \dot{\varepsilon}_p\ $
KKT conditions:	$\lambda \geq 0, \quad \phi(\Sigma_E, g) \leq 0, \quad \lambda \phi(\Sigma_E, g) = 0$
Boundary conditions for ε_p :	$\varepsilon_p \times n _{\partial\Omega} = 0, \quad (\text{Curl } \varepsilon_p)^T \times n _{\partial\Omega} = 0$

and for every $\beta \in L^2(\Omega)$, integrate (80) over Ω using the pair of functions (q, β) and get

$$\begin{aligned} \int_{\Omega} \mathcal{D}(q, \beta) dx &\geq \int_{\Omega} \mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p) dx + \int_{\Omega} [\langle \sigma + \Sigma_{\text{curl}} + \Sigma_{\text{inc}}, q - \dot{\varepsilon}_p \rangle + g(\beta - \dot{\gamma}_p)] dx \\ &= \int_{\Omega} [\langle \sigma - \mu L_c^2 \text{sym Curl}(\text{sym Curl } \varepsilon_p) - \mu \widehat{L}_c^4 \text{inc inc } \varepsilon_p, q - \dot{\varepsilon}_p \rangle \\ &\quad - \mu k_2 \gamma_p (\beta - \dot{\gamma}_p)] dx. \end{aligned} \quad (84)$$

Now integrating by parts the two terms $\langle \text{sym Curl}(\text{sym Curl } \varepsilon_p), q - \dot{\varepsilon}_p \rangle$ once and $\langle \text{inc inc } \varepsilon_p, q - \dot{\varepsilon}_p \rangle$ twice, using the boundary conditions

$$(q - \dot{\varepsilon}_p) \times n|_{\partial\Omega} = 0 \quad \text{and} \quad (\text{Curl}(q - \dot{\varepsilon}_p))^T \times n|_{\partial\Omega} = 0,$$

we obtain from (84) that

$$\begin{aligned} \int_{\Omega} \mathcal{D}(q, \beta) dx &\geq \int_{\Omega} \mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p) dx + \int_{\Omega} \langle \mathbb{C}_{\text{iso}}(\text{sym } \nabla u - \varepsilon_p), q - \dot{\varepsilon}_p \rangle dx \\ &\quad - \mu k_2 \int_{\Omega} \gamma_p (\beta - \dot{\gamma}_p) dx - \mu L_c^2 \int_{\Omega} \langle \text{sym Curl } \varepsilon_p, \text{sym Curl}(q - \dot{\varepsilon}_p) \rangle dx \\ &\quad - \mu \widehat{L}_c^4 \int_{\Omega} \langle \text{inc } \varepsilon_p, \text{inc}(q - \dot{\varepsilon}_p) \rangle dx. \end{aligned} \quad (85)$$

Adding (85) to the weak formulation of the equilibrium in (83), we obtain the weak formulation of our model of gradient plasticity with isotropic hardening and Kröner's incompatibility tensor

$$\begin{aligned} &\int_{\Omega} [\langle \mathbb{C}_{\text{iso}}(\text{sym } \nabla u - \varepsilon_p), (\text{sym } \nabla v - q) - (\text{sym } \nabla \dot{u} - \dot{\varepsilon}_p) \rangle + \mu k_2 \gamma_p (\beta - \dot{\gamma}_p) \\ &\quad + \mu L_c^2 \langle \text{sym Curl } \varepsilon_p, \text{sym Curl}(q - \dot{\varepsilon}_p) \rangle + \mu \widehat{L}_c^4 \langle \text{inc } \varepsilon_p, \text{inc}(q - \dot{\varepsilon}_p) \rangle] dx \\ &\quad + \int_{\Omega} \mathcal{D}(q, \beta) dx - \int_{\Omega} \mathcal{D}(\dot{\varepsilon}_p, \dot{\gamma}_p) dx \geq \int_{\Omega} f(v - \dot{u}) dx. \end{aligned} \quad (86)$$

That is,

$$a(w, z - \dot{w}) + j(z) - j(\dot{w}) \geq \langle \ell, z - \dot{w} \rangle, \quad (87)$$

where

$$a(w, z) := \int_{\Omega} \left[\langle \mathbb{C}_{\text{iso}}(\text{sym}(\nabla u - p)), \text{sym} \nabla v - q \rangle + \mu k_2 \gamma_p \beta + \mu L_c^2 \langle \text{sym Curl } \varepsilon_p, \text{sym Curl } q \rangle + \mu \widehat{L}_c^4 \langle \text{inc } \varepsilon_p, \text{inc } q \rangle \right] dx, \quad (88)$$

$$j(z) := \int_{\Omega} \mathcal{D}(q, \beta) dx, \quad (89)$$

$$\langle \ell, z \rangle := \int_{\Omega} f v dx, \quad (90)$$

for $w = (u, \varepsilon_p, \gamma_p)$ and $z = (v, q, \beta)$.

4.3.6. Existence result for the weak formulation.

We prove the existence result for the weak formulation (86) by closely following the approach by now classical, which uses the abstract machinery developed by Han and Reddy in [40] for mathematical problems in geometrically linear classical plasticity and used, for instance, in [16, 31, 32, 41, 42] and [103, 109, 130] for models of gradient plasticity. Precisely, we will need the following theorem.

Theorem 4.2. (Han and Reddy [40, Theorem 6.19]). *Let \mathbf{Z} be a Hilbert space and let \mathbf{W} be a non-empty closed convex subset of \mathbf{Z} . Consider the following problem: find $w \in \mathbf{H}^1([0, T]; \mathbf{Z})$ with $w(0) = 0$ such that for almost every $t \in [0, T]$, $\dot{w}(t) \in \mathbf{W}$ and*

$$a(w, z - \dot{w}) + j(z) - j(\dot{w}) \geq \langle \ell, z - \dot{w} \rangle \text{ for every } z \in \mathbf{W}. \quad (91)$$

Assume that the following hold:

1. the bilinear form a is symmetric, continuous on \mathbf{Z} and coercive on \mathbf{W} , i.e. there exist $C > 0$ and $\alpha > 0$ such that

$$a(w, z) \leq C \|w\|_{\mathbf{Z}} \|z\|_{\mathbf{Z}} \quad \forall w, z \in \mathbf{Z} \quad \text{and} \quad a(z, z) \geq \alpha \|z\|_{\mathbf{Z}}^2 \quad \forall z \in \mathbf{W}; \quad (92)$$

2. $\ell \in \mathbf{H}^1([0, T]; \mathbf{Z}')$ with $\ell(0) = 0$;
3. the functional j is non-negative, convex, lower continuous and positively 1-homogeneous on \mathbf{Z} , i.e. $j(sz) = |s|j(z) \quad \forall s \in \mathbb{R}, \quad \forall z \in \mathbf{Z}$.

Then the problem (91) has a solution $w \in \mathbf{H}^1([0, T]; \mathbf{Z})$.

Therefore, the problem is then reduced to finding a suitable Hilbert space \mathbf{Z} and its subset \mathbf{W} such that the bilinear form $a(\cdot, \cdot)$ and the functionals j and ℓ satisfy the assumptions of Theorem 4.2.

The choices of function spaces for the displacement variable u and the isotropic hardening variable γ_p are straightforward as

$$u \in \mathbf{H}_0^1(\Omega, \mathbb{R}^3) \quad \text{and} \quad \gamma_p \in \mathbf{L}^2(\Omega).$$

For the plastic strain variable ε_p , we first need to introduce the space

$$\begin{aligned} \mathbf{H}_{\text{inc}}(\text{Curl}, \Omega; \mathfrak{sl}(3) \cap \text{Sym}(3)) &:= \{q \in \mathbf{L}^2(\Omega, \mathfrak{sl}(3) \cap \text{Sym}(3)) \mid (\text{Curl } q)^{\text{T}} \in \mathbf{H}(\text{Curl}, \Omega; \mathbb{R}^{3 \times 3})\} \\ &:= \{q \in \mathbf{H}(\Omega, \mathfrak{sl}(3) \cap \text{Sym}(3)) \mid \text{inc } q \in \mathbf{L}^2(\text{Curl}, \Omega; \mathbb{R}^{3 \times 3})\} \end{aligned} \quad (93)$$

equipped with the norm

$$\begin{aligned} \|q\|_{\text{inc}}^2 &:= \|q\|_{\mathbf{L}^2(\Omega)}^2 + \|(\text{Curl } q)^{\text{T}}\|_{\mathbf{H}(\text{Curl}; \Omega)}^2 = \|q\|_{\mathbf{L}^2}^2 + \|(\text{Curl } q)^{\text{T}}\|_{\mathbf{L}^2}^2 + \|\text{Curl}[(\text{Curl } q)^{\text{T}}]\|_{\mathbf{L}^2}^2 \\ &= \|q\|_{\mathbf{H}(\text{Curl}; \Omega)}^2 + \|\text{inc } q\|_{\mathbf{L}^2(\Omega)}^2. \end{aligned} \quad (94)$$

Let us mention that spaces of functions involving the inc-operator were already used in the literature and we refer the interested reader, for instance, to the papers [60, 76].

We also consider the closure $\mathbf{H}_{\text{sym, inc}}(\text{Curl}, \Omega, \partial\Omega; \mathfrak{sl}(3) \cap \text{Sym}(3))$ of the linear subspace

$$\left\{ q \in C^\infty(\overline{\Omega}, \text{Sym}(3)) \mid \text{tr } q = 0, \quad q \times n|_{\partial\Omega} = 0 \text{ and } (\text{Curl } q)^T \times n|_{\partial\Omega} = 0 \right\}$$

in the norm

$$\|q\|_{\text{symcurl, inc}}^2 := \|q\|_{L^2}^2 + \|\text{sym Curl } q\|_{L^2}^2 + \|\text{inc } q\|_{L^2}^2. \quad (95)$$

Motivated by the well-posedness question for models of infinitesimal gradient plasticity (especially for models dictated by invariance under infinitesimal rotations) [16, 31, 77–79], infinitesimal Cosserat elasticity [74, 80, 81], infinitesimal Cosserat elasto-plasticity [82–85] and infinitesimal relaxed micromorphic [86–88], Bauer et al. [89, 90] (see also Neff et al. [91–94]) derived a new inequality extending Korn's first inequality to incompatible tensor fields, namely there exists a constant $C(\Omega) > 0$ such that

$$\begin{aligned} \forall X \in \mathbf{H}(\text{Curl}; \Omega, \mathbb{R}^{3 \times 3}), \quad X \times n|_{\partial\Omega} = 0 : \\ \|X\|_{L^2(\Omega)} \leq C(\Omega) \left(\|\text{sym } X\|_{L^2(\Omega)} + \|\text{Curl } X\|_{L^2(\Omega)} \right). \end{aligned} \quad (96)$$

Now, if we apply the incompatible Korn-type inequality to $X = (\text{Curl } q)^T$ for $q \in C^\infty(\overline{\Omega}, \text{Sym}(3))$ with $(\text{Curl } q)^T \times n|_{\partial\Omega} = 0$, we obtain

$$\begin{aligned} \|\text{Curl } q\|_{L^2(\Omega)} &= \|(\text{Curl } q)^T\|_{L^2(\Omega)} \\ &\leq C(\Omega) \left(\left\| \text{sym} \left((\text{Curl } q)^T \right) \right\|_{L^2(\Omega)} + \|\text{Curl} [(\text{Curl } \varepsilon_p)^T]\|_{L^2(\Omega)} \right) \\ &= C(\Omega) \left(\|\text{sym Curl } q\|_{L^2(\Omega)} + \|\text{inc } q\|_{L^2(\Omega)} \right), \end{aligned} \quad (97)$$

then we have the decisive identity

$$\begin{aligned} \mathbf{H}_{\text{sym, inc}}(\text{Curl}, \Omega, \partial\Omega; \mathfrak{sl}(3) \cap \text{Sym}(3)) \\ \equiv \{ q \in \mathbf{H}_0(\text{Curl}, \Omega, \partial\Omega; \mathfrak{sl}(3) \cap \text{Sym}(3)), \quad (\text{Curl } q)^T \in \mathbf{H}_0(\text{Curl}, \Omega, \partial\Omega; \mathbb{R}^{3 \times 3}) \} \\ = \{ q, (\text{Curl } q)^T \in \mathbf{H}(\text{Curl}, \Omega, \mathbb{R}^{3 \times 3}), \quad \text{tr } q = 0 \text{ a.e. in } \Omega, \quad q \times n|_{\partial\Omega} = (\text{Curl } q)^T \times n|_{\partial\Omega} = 0 \} \end{aligned} \quad (98)$$

with the norms $\|\cdot\|_{\text{inc}}$ and $\|\cdot\|_{\text{symcurl, inc}}$ being equivalent.

Now, we set

$$\mathbf{V} := \mathbf{H}_0^1(\Omega; \mathbb{R}^3), \quad (99)$$

$$\mathbf{Q} := \{ q \in \mathbf{H}_{\text{inc}}(\text{Curl}, \Omega; \mathfrak{sl}(3) \cap \text{Sym}(3)) \mid q \times n|_{\partial\Omega} = 0 \text{ and } (\text{Curl } q)^T \times n|_{\partial\Omega} = 0 \}, \quad (100)$$

$$\mathbf{\Lambda} := L^2(\Omega), \quad (101)$$

$$\mathbf{Z} := \mathbf{V} \times \mathbf{Q} \times \mathbf{\Lambda}, \quad (102)$$

$$\mathbf{W} := \{ z = (v, q, \beta) \in \mathbf{Z} \mid \|q\| \leq \beta \}, \quad (103)$$

equipped with the norms

$$\begin{aligned} \|v\|_{\mathbf{V}} &:= \|\nabla v\|_{L^2(\Omega)}, \quad \|q\|_{\mathbf{Q}} := \|q\|_{\text{inc}}, \quad \|\beta\|_{\mathbf{\Lambda}} = \|\beta\|_{L^2(\Omega)}, \\ \|z\|_{\mathbf{Z}}^2 &:= \|v\|_{\mathbf{V}}^2 + \|q\|_{\mathbf{Q}}^2 + \|\beta\|_{\mathbf{\Lambda}}^2 \quad \text{for } z = (v, q, \beta) \in \mathbf{Z}. \end{aligned} \quad (104)$$

Let us prove the coercivity of the bilinear form $a(\cdot, \cdot)$ on the closed convex set \mathbf{W} , where the constraint $\|q\| \leq \beta$ in \mathbf{W} plays a crucial role. Let, therefore, $z = (v, q, \beta) \in \mathbf{W}$. Then,

$$\begin{aligned}
a(z, z) &\geq m_0 \|\text{sym}(\nabla v) - q\|_2^2 + \mu k_2 \|\beta\|_{L^2}^2 + \mu L_c^2 \|\text{sym Curl } q\|_2^2 + \mu \widehat{L}_c^4 \|\text{inc } q\|_{L^2}^2 \\
&\quad (m_0 > 0 \text{ is from (29)}) \\
&= m_0 \left[\|\text{sym}(\nabla v)\|_2^2 + \|q\|_{L^2}^2 - 2\langle \text{sym}(\nabla v), q \rangle \right] + \mu k \|\beta\|_{L^2}^2 \\
&\quad + \mu L_c^2 \|\text{sym Curl } q\|_2^2 + \mu \widehat{L}_c^4 \|\text{inc } q\|_{L^2}^2 \\
&\geq m_0 \left[\|\text{sym}(\nabla v)\|_{L^2}^2 + \|q\|_{L^2}^2 - \theta \|\text{sym}(\nabla v)\|_{L^2}^2 - \frac{1}{\theta} \|q\|_{L^2}^2 \right] + \frac{1}{2} \mu k_2 \|\beta\|_2^2 \\
&\quad + \frac{1}{2} \mu k_2 \|q\|_{L^2}^2 + \mu L_c^2 \|\text{sym Curl } q\|_{L^2}^2 + \mu \widehat{L}_c^4 \|\text{inc } q\|_{L^2}^2 \\
&\quad (\text{using Young's inequality and } \|q\| \leq \beta \text{ from } W) \\
&= m_0(1 - \theta) \|\text{sym}(\nabla v)\|_2^2 + \left[m_0 \left(1 - \frac{1}{\theta} \right) + \frac{1}{2} \mu k_2 \right] \|q\|_2^2 + \frac{1}{2} \mu k_2 \|\beta\|_2^2 \\
&\quad + \mu L_c^2 \|\text{sym Curl } q\|_{L^2}^2 + \mu \widehat{L}_c^4 \|\text{inc } q\|_{L^2}^2.
\end{aligned}$$

Thus, choosing θ such that $\frac{2m_0}{2m_0 + \mu k_2} \leq \theta < 1$, and using the classical Korn's first inequality, there exists some positive constant $K(m_0, \mu, k_2, \Omega) > 0$ such that

$$\begin{aligned}
a(z, z) &\geq K \left[\|v\|_V^2 + \|q\|_{L^2}^2 + \|\beta\|_\Lambda^2 + \mu L_c^2 \|\text{sym Curl } q\|_{L^2}^2 + \mu \widehat{L}_c^4 \|\text{inc } q\|_{L^2}^2 \right] \\
&\geq C \left[\|v\|_V^2 + \|q\|_Q^2 + \|\beta\|_\Lambda^2 \right] = C \|z\|_Z^2 \quad \forall z = (v, q, \beta) \in W,
\end{aligned} \tag{105}$$

where $C = C(m_0, \mu, k_2, \Omega, L_c, \widehat{L}_c) > 0$. For the second inequality in (105), we used the inequality (97) obtained as a consequence of the Korn-type inequality for incompatible tensor fields in Neff et al. [91–94]. \square

Thus, assuming that the body is initially unloaded and undeformed, which corresponds to assuming that $f(x, 0) = 0$ for almost all $x \in \Omega$ with homogeneous initial conditions, we obtained the following existence result for the weak formulation (86) of our model.

Theorem 4.3. *Under the choices of the Hilbert space \mathbf{Z} and the closed convex subset \mathbf{W} in (99)–(103) with the norms in (104) and the functionals a , j and ℓ in (88)–(90), the weak formulation (86) when written as the variational inequality of the second kind (91) has a solution $w = (u, \varepsilon_p, \gamma_p)$ in $H^1([0, T]; \mathbf{Z})$ with $\dot{w} \in L^2([0, T]; \mathbf{W})$.*

Remark 4.2. Uniqueness of the strong solution is obtained as in [33] provided the following further assumptions are satisfied:

$$\begin{aligned}
\text{sym Curl}(\text{sym Curl } \varepsilon_p) &\in L^2(\Omega, \text{Sym}(3) \cap \mathfrak{sl}(3)) \\
\text{Curl}([\text{Curl Curl}[\text{Curl } \varepsilon_p]^T]^T) &\in L^2(\Omega, \mathbb{R}^{3 \times 3}).
\end{aligned} \tag{106}$$

5. Discussion

It remains a difficult task to reconcile mathematical and physical requirements. Indeed, the incorporation of Kröner's incompatibility tensor $\text{inc } \varepsilon_p$ is physically transparent and the novel model is micro-random and gauge-invariant. Micro-randomness is useful for polycrystals and gauge-invariance is a generally physically necessary requirement. However, using integration by parts in order to arrive at a global reduced dissipation inequality, the following lowest-order boundary conditions

$$\varepsilon_p \times n|_{\partial\Omega} = 0 \quad \text{and} \quad (\text{Curl } \varepsilon_p)^T \times n|_{\partial\Omega} = 0 \tag{107}$$

impose themselves.

From a mathematical point of view these expressions are, however, not well-defined as boundary traces through a control of the given free energy. In order to give them a well-defined meaning, we resorted to adding an additional term in the free energy, namely

$$\frac{1}{2} \mu L_c^2 \|\operatorname{dev} \operatorname{sym}(\operatorname{Curl} \varepsilon_p)^T\|^2 = \frac{1}{2} \mu L_c^2 \|\operatorname{sym}(\operatorname{Curl} \varepsilon_p)^T\|^2,$$

the equality here is due to the fact that $\operatorname{tr}(\operatorname{Curl} S) = 0$ forever. This term provides the missing boundary control for (107) by the Korn-type inequality for incompatible tensor fields in [89–94]. However, the additional term breaks the gauge-invariance of the model, while it satisfies the micro-randomness condition.

On the positive side, the invariance under the diffeomorphism group (gauge-invariance) is replaced by the invariance under infinitesimal conformal group (both statements adapted to our geometrically linear setting).

At the moment, we do not know how to set up a theory that is fully gauge-invariant and micro-random, while at the same time being mathematically well-posed. Consider, e.g., a model with plastic spin and add $\frac{1}{2} \mu L_c^2 \|\operatorname{Curl} p\|^2$ (see Table 6). This choice does not provide any control of $\|\operatorname{Curl} \operatorname{sym} p\|^2 = \|\operatorname{Curl} \varepsilon_p\|^2$ necessary for well-posedness of (107).

A preliminary conclusion could be that the micro-randomness assumption, which effectively reduces the flow law to the six-dimensional space of symmetric plastic strains ε_p , is to be critically seen in gradient plasticity approaches which are also supposed to satisfy gauge-invariance.

Notes

1. Cf. e.g. Hill [9, p. 30].
2. Aifantis wrote in [6, p. 218]: “...In conformity with established results - that the plastic strain rate $\dot{\varepsilon}_p$ is a state variable, rather than the strain ε_p itself.”
3. The plastic spin in the finite deformation flow theory of plasticity is defined as the skew-symmetric part of the so-called plastic distortion rate, i.e. $W_p := \operatorname{skew}(\dot{F}_p F_p^{-1})$, whereas its counterpart in the small strain theory is simply $\operatorname{skew}(\dot{p})$, where p is the non-symmetric infinitesimal plastic distortion.
4. The PMPD, which was derived independently in classical infinitesimal theory of plasticity from the so-called Drucker’s postulate by von Mises [35], Taylor [36], Hill [37] and Mandel [38] (and later as a consequence of Il’iushin’s postulate of plasticity in strain space) has the form $\langle \sigma - \sigma^*, \dot{\varepsilon}_p \rangle \geq 0$, where σ is the actual stress tensor, $\dot{\varepsilon}_p$ is the plastic strain-rate tensor and σ^* is any admissible stress tensor. The PMPD is equivalent to the associated flow rule in the dual formulation in the local theory of plasticity. The maximal dissipation (associated flow rule) simplifies the modelling framework and facilitates the mathematical treatment.
5. Note that \mathcal{R}_{jkl}^i is both geometrically and physically nonlinear.
6. The role of that tensor has been critically discussed by Acharya [63].
7. Note that Gurtin uses a different definition of the Curl operator. We have the relation $\operatorname{Curl} F_p = [\operatorname{Curl}_{\text{Gurtin}} F_p]^T$ (see [22]).
8. Only time-objectivity requirements are not to be discussed.
9. Rotating grains against each other (see Neff et al. [71]) in a polycrystal changes the eigen-stresses along grain boundaries. Therefore, our new invariance requirement cannot be a fundamental law of nature but may rather serve to concentrate on some effective macroscopic features in a homogenized model.


Acknowledgements

We thank David J. Steigmann (University of Berkeley) for inspiring discussions on invariance conditions in plasticity theory which motivated us to introduce our micro-randomness condition and to consider the fourth-order gradient plasticity model for polycrystals. The first author thanks the Faculty of Mathematics of the University of Duisburg-Essen (Germany) for its kind hospitality during his visit in April 2017.

Funding

The author(s) received no financial support for the research, authorship, and/or publication of this article.

ORCID iD

François Ebobisse  <http://orcid.org/0000-0001-6863-8017>

References

- [1] Fleck, NA, and Hutchinson, JW. Strain gradient plasticity. *Adv Appl Mech* 1997; 33: 295–361.
- [2] Fleck, NA, Müller, GM, Ashby, MF, and Hutchinson, JW. Strain gradient plasticity: Theory and experiment. *Acta Metall Mater* 1994; 42: 475–487.
- [3] Nix, WD and Gao, H. Indentation size effects in crystalline materials: A law for strain gradient plasticity. *J Mech Phys Solids* 1998; 46: 411–425.
- [4] Stölken, JS, and Evans, AG. A microbend test method for measuring the plasticity length scale. *Acta Mater* 1998; 46: 5109–5115.
- [5] Aifantis, EC. On the microstructural origin of certain inelastic models. *ASME J Eng Mater Technol* 1984; 106: 326–330.
- [6] Aifantis, EC. The physics of plastic deformation. *Int J Plasticity*, 3:211–247, 1987.
- [7] Mühlhaus, HB, and Aifantis, E. A variational principle for gradient plasticity. *Int J Solids Struct* 1991; 28(7): 845–853.
- [8] Zbib, HM, and Aifantis, EC. On the gradient-dependent theory of plasticity and shear banding. *Acta Mechanica* 1992; 92: 209–225.
- [9] Hill, R. *The Mathematical Theory of Plasticity*. New York: Oxford University Press, 1950.
- [10] Fleck, NA, and Hutchinson, JW. A reformulation of strain gradient plasticity. *J Mech Phys Solids* 2001; 49: 2245–2271.
- [11] Gudmundson, P. A unified treatment of strain gradient plasticity. *J Mech Phys Solids* 2004; 52: 1379–1406.
- [12] Gurtin, ME, and Anand, L. Thermodynamics applied to gradient theories involving the accumulated plastic strain: The theories of Aifantis and Fleck and Hutchinson and their generalization. *J Mech Phys Solids* 2009; 57: 405–421.
- [13] Acharya, A, and Bassani, JL. Lattice incompatibility and a gradient theory of crystal plasticity. *J Mech Phys Solids* 2000; 48(8): 1565–1595.
- [14] Cermelli, P, and Gurtin, ME. On the characterization of geometrically necessary dislocations in finite plasticity. *J Mech Phys Solids* 2001; 49: 1539–1568.
- [15] Gurtin, ME, and Anand, L. A theory of strain gradient plasticity for isotropic, plastically irrotational materials. Part II: Finite deformation. *Int J Plasticity* 2005; 21(12): 2297–2318.
- [16] Neff, P, Chelmiński, K, and Alber, HD. Notes on strain gradient plasticity. Finite strain covariant modelling and global existence in the infinitesimal rate-independent case. *Math Mod Meth Appl Sci* 2009; 19(2): 1–40.
- [17] Gurtin, ME, and Anand, L. A theory of strain gradient plasticity for isotropic, plastically irrotational materials. Part I: Small deformations. *J Mech Phys Solids* 2005; 53: 1624–1649.
- [18] Gurtin, ME, and Reddy, BD. Gradient single-crystal plasticity within a von Mises–Hill framework based on a new formulation of self- and latent-hardening relations. *J Mech Phys Solids* 2014; 68: 134–160.
- [19] Menzel, M, and Steinmann, P. On the formulation of higher gradient plasticity for single and polycrystals. *J Phys France* 1998; 8: 239–247.
- [20] Menzel, M, and Steinmann, P. On the continuum formulation of higher gradient plasticity for single and polycrystals. *J Mech Phys Solids* 2000; 48: 1777–1796. Erratum: 2001; 49: 1179–1180.
- [21] Svendsen, B, Neff, P, and Menzel, A. On constitutive and configurational aspects of models for gradient continua with microstructure. *Z Angew Math Mech* 2009; 89(8): 687–697.
- [22] Gurtin, ME, Fried, E, and Anand, L. *The Mechanics and Thermodynamics of Continua*. Cambridge: Cambridge University Press, 2010.
- [23] Dafalias, YF. The plastic spin. *J Appl Mech* 1985; 52: 865–871.
- [24] Kratochvíl, J. On a finite strain theory of elastic–inelastic materials. *Acta Mech* 1973; 16: 127–142.
- [25] Mandel, J. Equations constitutives et directeurs dans les milieux plastiques et viscoplastiques. *Int J Solids Struct* 1973; 9: 725–740.
- [26] Bardella, L. A comparison between crystal and isotropic strain gradient plasticity theories with accent on the role of the plastic spin. *Eur J Mech A/Solids* 2009; 28(3): 638–646.
- [27] Poh, LH. Scale transition of a higher order plasticity model - A consistent homogenization theory from meso to macro. *J Mech Phys Solids* 2013; 61: 2692–2710.
- [28] Bardella, L, and Panteghini, A. Modelling the torsion of thin metal wires by distortion gradient plasticity. *J Mech Phys Solids* 2015; 78: 467–492.
- [29] Bardella, L. Size effects in phenomenological strain gradient plasticity constitutively involving the plastic spin. *Int J Eng Sci* 2010; 48(5): 550–568.
- [30] Gurtin, ME. A gradient theory of small deformation isotropic plasticity that accounts for the Burgers vector and for dissipation due to plastic spin. *J Mech Phys Solids* 2004; 52: 2545–2568.
- [31] Ebobisse, F, and Neff, P. Existence and uniqueness in rate-independent infinitesimal gradient plasticity with isotropic hardening and plastic spin. *Math Mech Solids* 2010; 15: 691–703.
- [32] Ebobisse, F, Neff, P and Reddy, BD. Existence results in dislocation based rate-independent isotropic gradient plasticity with kinematic hardening and plastic spin: The case with symmetric local backstress. *Preprint <http://arxiv.org/pdf/1504.01973.pdf>*.
- [33] Ebobisse, F, Hackl, K, and Neff, P. A canonical rate-independent model of geometrically linear isotropic gradient plasticity with isotropic hardening and plastic spin accounting for the Burgers vector. *Continuum Mech Thermodyn* 2019; 31: 1477–1502 <https://doi.org/10.1007/s00161-019-00755-5>

- [34] Mielke, A, and Stefanelli, U. Linearized plasticity is the evolutionary Γ -limit of finite plasticity. *J Eur Math Soc* 2013; 15(3): 923–948.
- [35] von Mises, R. Mechanik der plastischen Formänderung von Kristallen. *Z Angew Math Mech* 1928; 8: 161.
- [36] Taylor, GI. A connection between the criterion of yield and the strain-ratio relationship in plastic solids. *Proc Roy Soc A* 1947; 191: 441–446.
- [37] Hill, R. A variational principle of maximum plastic work in classical plasticity. *Quart J Mech Appl Math* 1948; 1(1): 18–28.
- [38] Mandel, J. Contribution théorique à l'étude de l'écroutissage des lois de l'écoulement plastique. In: *Proceedings of the 11th International Congress on Applied Mechanics*, pp. 502–509, 1964.
- [39] Moreau, JJ. Application of convex analysis to the treatment of elastoplastic systems. In Germain, P and Nayroles, B (eds.) *Applications of Methods of Functional Analysis to Problems in Mechanics*. Berlin: Springer-Verlag, 1976.
- [40] Han, W, and Reddy, BD. *Plasticity: Mathematical Theory and Numerical Analysis*. New York: Springer-Verlag, 1999.
- [41] Djoko, JK, Ebobisse, F, McBride, AT and Reddy, BD. A discontinuous Galerkin formulation for classical and gradient plasticity. Part 1: Formulation and analysis. *Comput Meth Appl Mech Engng* 2007; 196: 3881–3897.
- [42] Reddy, BD, Ebobisse, F, and McBride, A. Well-posedness of a model of strain gradient plasticity for plastically irrotational materials. *Int J Plasticity* 2008; 24: 55–73.
- [43] Ebobisse, F, McBride, AT, and Reddy, BD. On the mathematical formulations of a model of gradient plasticity. In Reddy, BD (ed.) *IUTAM-Symposium on Theoretical, Modelling and Computational Aspects of Inelastic Media*, Cape Town, 2008, pp. 117–128. Berlin: Springer, 2008.
- [44] Ebobisse, F, Neff, P, and Aifantis, EC. Existence result for a dislocation based model of single crystal gradient plasticity with isotropic or linear kinematic hardening. *Quart J Mech Appl Math* 2018; 71: 99–124.
- [45] Ebobisse, F, Neff, P, and Forest, S. Well-posedness for the microcurl model in both single and polycrystal gradient plasticity. *Int J Plasticity* 2018 107: 1–26.
- [46] Krishnan, J, and Steigmann, DJ. A polyconvex formulation of isotropic elastoplasticity. *IMA J Appl Math* 2014; 79: 722–738.
- [47] Kröner, E. Der fundamentale Zusammenhang zwischen Versetzungsdichte und Spannungsfunktion. *Z Phys* 1955; 142: 463–475.
- [48] Kröner, E. Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen. *Arch Ration Mech Anal* 1960; 4: 273–334.
- [49] Kondo, K. Non-Riemannian geometry of imperfect crystals from a macroscopic viewpoint. In: Kondo, K (ed.) *RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Science by Means of Geometry*, vol. 1, pp. 6–17. Tokyo: Gakujutsu Bunken Fukyu-Kai, 1955.
- [50] Van Goethem, N. Strain incompatibility in single crystals: Kröner's formula revisited. *J Elasticity* 2011; 103: 95–111.
- [51] Van Goethem, N. Dislocation-induced linear-elastic strain dynamics by a Cahn–Hilliard-type equation. *Math Mech Complex Syst* 2016; 4(2): 169–195.
- [52] Van Goethem, N. Front migration for the dislocation strain in single crystals. *Comm Math Sci* 2017; 15(7): 1843–1866.
- [53] De Wit, R. A view of the relation between the continuum theory of lattice defects and non-Euclidean geometry in the linear approximation. *Int J Engng Sci* 1981; 19: 1475–1506.
- [54] Lanczos, C. A remarkable property of the Riemann–Christoffel tensor in four dimensions. *Ann Math* 1938; 39(4): 842–850.
- [55] Ghiba, I-D, Neff, P, Madeo, A, and Münch, I. A variant of the linear isotropic indeterminate couple stress model with symmetric local force-stress, symmetric nonlocal force-stress, symmetric couple-stresses and complete traction boundary conditions. *Math Mech Solids* 2017; 22(6): 1221–1266.
- [56] Ciarlet, PhG, and Laurent, F. Continuity of deformation as a function of its Cauchy–Green tensor. *Arch Rat Mech Anal* 2003; 167(3): 255–269.
- [57] Marsden, JE, and Hughes, JR. *Mathematical Foundations of Elasticity*. Englewood Cliffs, NJ: Prentice-Hall, 1983.
- [58] Ciarlet, PhG. *An Introduction to Differential Geometry with Applications to Elasticity*. Berlin: Springer-Verlag, 2005.
- [59] Maggiani, GB, Scala, R, and Van Goethem, N. A compatible–incompatible decomposition of symmetric tensors in L_p with applications in elasticity. *Math Meth Appl Sci* 2015; 38(18): 5217–5230.
- [60] Amstutz, S, and Van Goethem, N. Analysis of the incompatibility operator and application in intrinsic elasticity with dislocations. *SIAM J Math Anal* 2015; 48(1): 320–349.
- [61] Davini, C and Parry, GP. On defect preserving deformations in crystals. *Int J Plasticity* 1989; 5: 337–369.
- [62] Epstein, M. *The Geometrical Language of Continuum Mechanics*. Cambridge: Cambridge University Press, 2010.
- [63] Acharya, A. A counterpoint to Cermelli and Gurtin's criteria for choosing the "correct" geometric dislocation tensor in finite plasticity. In Reddy, BD (ed.) *IUTAM-Symposium on Theoretical, Modelling and Computational Aspects of Inelastic Media*, Cape Town, 2008, pp. 99–105. Berlin: Springer, 2008.
- [64] Berdichevsky, VL and Sedov, LI. Dynamic theory of continuously distributed dislocations. Its relation to plasticity theory. *PMM* 1967; 31(6): 981–1000 (English translation: *J Appl Math Mech (PMM)* 1967; 31(6): 989–1006).
- [65] Berdichevsky, VL. Continuum theory of dislocations revisited. *Cont Mech Thermodyn* 2006; 18: 195–222.
- [66] Hay, GE. *Vector and Tensor Analysis*. New York: Dover, 1953.
- [67] Svendsen, B. Continuum thermodynamic models for crystal plasticity including the effects of geometrically necessary dislocations. *J Mech Phys Solids* 2002; 50(25): 1297–1329.
- [68] Lazar, M. Dislocation theory as a 3-dimensional translation gauge theory. *Ann Phys (Leipzig)* 2000; 9: 461–473.
- [69] Lazar, M. An elastoplastic theory of dislocations as a physical field theory with torsion. *J Phys A: Math Gen* 2002; 35: 1983–2004.
- [70] Lazar, M and Anastassiadis, C. The gauge theory of dislocations: Conservation and balance laws. *Phil Mag* 2008; 88: 1673–1699.

- [71] Neff, P, Jeong, J and Ramézani, H. Subgrid interaction and micro-randomness - Novel invariance requirements in infinitesimal gradient plasticity. *Int J Solids Struct* 2009; 46: 4261–4276.
- [72] Münch, I, and Neff, P. Rotational invariance conditions in elasticity, gradient elasticity and its connection to isotropy. *Math Mech Solids* 2016; 15: 1–40.
- [73] Neff, P, Ghiba, I-D, Madeo, A, Placidi, L, and Rosi, G. A unifying perspective: The relaxed linear micromorphic continuum. *Cont Mech Thermodyn* 2014; 26: 639–681.
- [74] Neff, P, and Jeong, J. A new paradigm: The linear isotropic Cosserat model with conformally invariant curvature energy. *Z Angew Math Mech* 2009; 89(2): 107–122.
- [75] Nabarro, FRN. *Theory of Crystal Dislocations*. Oxford: Oxford University Press, 1967.
- [76] Amstutz, S, and Van Goethem, N. Incompatibility-governed elasto-plasticity for continua with dislocations. *Proc R Soc A* 2017; 473(2199): 20160734.
- [77] Nesenenko, S, and Neff, P. Well-posedness for dislocation based gradient visco-plasticity I: Subdifferential case. *SIAM J Math Anal* 2012; 44(3): 1695–1712.
- [78] Nesenenko, S, and Neff, P. Well-posedness for dislocation based gradient visco-plasticity II: General non-associative monotone plastic flow. *Math Mech Complex Syst* 2013; 1(2): 149–176.
- [79] Neff, P, Sydow, A, and Wieners, C. Numerical approximation of incremental infinitesimal gradient plasticity. *Int J Num Meth Engng* 2009; 77(3): 414–436.
- [80] Jeong, J, and Neff, P. Existence, uniqueness and stability in linear Cosserat elasticity for weakest curvature conditions. *Math Mech Solids* 2010; 15(1): 78–95.
- [81] Neff, P. The Cosserat couple modulus for continuous solids is zero viz the linearized Cauchy-stress tensor is symmetric. *Z Angew Math Mech* 2006; 86: 892–912.
- [82] Neff, P, and Chelmiński, K. Infinitesimal elastic–plastic Cosserat micropolar theory. Modelling and global existence in the rate-independent case. *Proc Roy Soc Edinb A* 2005; 135: 1017–1039.
- [83] Neff, P, and Knees, D. Regularity up to the boundary for nonlinear elliptic systems arising in time-incremental infinitesimal elasto-plasticity. *SIAM J Math Anal* 2008; 40(1): 21–43.
- [84] Chelmiński, K, and Neff, P. A note on approximation of Prandtl–Reuss plasticity through Cosserat-plasticity. *Quart Appl Math* 2008; 66(2): 351–357.
- [85] Neff, P, Chelmiński, K, Müller, W, and Wieners, C. A numerical solution method for an infinitesimal elastic–plastic Cosserat model. *Math Mod Meth Appl Sci* 2007; 17(8): 1211–1239.
- [86] Neff, P, Ghiba, I-D, Lazar, M, and Madeo, A. The relaxed linear micromorphic continuum: well-posedness of the static problem and relations to the gauge theory of dislocations. *Quart J Mech Appl Math* 2015; 68: 53–84.
- [87] Neff, P, Jeong, J, Münch, I, and Ramezani, H. Mean field modeling of isotropic random Cauchy elasticity versus microstretch elasticity. *Z Angew Math Phys* 2009; 60(3): 479–497.
- [88] Neff, P. Existence of minimizers for a finite-strain micromorphic elastic solid. *Proc Roy Soc Edinb A* 2006; 136: 997–1012.
- [89] Bauer, S, Neff, P, Pauly, D, and Starke, G. New Poincaré-type inequalities, *C R Math* 2014; 352(4): 163–166.
- [90] Bauer, S, Neff, P, Pauly, D, and Starke, G. Dev-Div-and DevSym-devCurl-inequalities for incompatible square square tensor fields with mixed boundary conditions. *ESAIM Control Optim Calc Var* 2016; 22(1): 112–133.
- [91] Neff, P, Pauly, D, and Witsch, KJ. On a canonical extension of Korn’s first and Poincaré’s inequalities to $H(\text{Curl})$ motivated by gradient plasticity with plastic spin. *C R Math* 2011; 349(23–24): 1251–1254.
- [92] Neff, P, Pauly, D, and Witsch, KJ. On a canonical extension of Korn’s first and Poincaré’s inequalities to $H(\text{Curl})$. *J Math Sci (NY)* 2012; 185(5): 721–727.
- [93] Neff, P, Pauly, D, and Witsch, KJ. Maxwell meets Korn: A new coercive inequality for tensor fields with square integrable exterior derivatives. *Math Meth Appl Sci* 2012; 35(1): 65–71.
- [94] Neff, P, Pauly, D, and Witsch, KJ. Poincaré meets Korn via Maxwell: Extending Korn’s first inequality to incompatible tensor fields. *J Diff Equ* 2014; 258(4): 1267–1302.
- [95] Aifantis, EC. On the role of gradients in the localization of deformation and fracture. *Int J Engng Sci* 1992; 30: 1279–1299.
- [96] Aifantis, EC. Gradient plasticity. In: Lemaitre, J (ed.) *Handbook of Materials Behavior Models*, pp. 281–297. New York: Academic Press, 2001.
- [97] Aifantis, EC. Update on a class of gradient theories. *Mech Mater* 2003; 35: 259–280.
- [98] Aifantis, EC. Gradient material mechanics: Perspectives and prospects. *Acta Mech* 2014; 225: 999–1012.
- [99] Alber, HD. *Materials with Memory. Initial-Boundary Value Problems for Constitutive Equations with Internal Variables (Lecture Notes in Mathematics, vol. 1682)*. Berlin: Springer, 1998.
- [100] Anand, L, Gurtin, ME and Reddy, BD. The stored energy of cold work, thermal annealing, and other thermodynamic issues in single crystal plasticity at small length scales. *Int J Plasticity* 2015; 64: 1–25.
- [101] Bardella, L. A deformation theory of strain gradient crystal plasticity that accounts for geometrically necessary dislocations. *J Mech Phys Solids* 2006; 54: 128–160.
- [102] Bardella, L. Some remarks on the strain gradient crystal plasticity modelling, with particular reference to the material length scale involved. *Int J Plasticity* 2007; 23: 296–322.
- [103] Bargmann, S, Reddy, BD, and Klusemann, B. A computational study of a model of single-crystal strain gradient viscoplasticity with a fully-interactive hardening relation. *Int J Solids Struct* 2014; 51(15–16): 2754–2764.

- [104] Basak, A, and Gupta, A. Plasticity in multi-phase solids with incoherent interfaces and junctions. *Cont Mech Therm* 2016; 28(1–2): 423–442.
- [105] Basak, A, and Gupta, A. Influence of a mobile incoherent interface on the strain-gradient plasticity of a thin slab. *Int J Solid Struct* 2017; 108: 126–138.
- [106] Bertram, A. An alternative approach to finite plasticity based on material isomorphism. *Int J Plasticity* 1998; 52: 353–374.
- [107] Casey, J. A convenient form of the multiplicative decomposition of the deformation gradient. *Math Mech Solids* 2016; 22(3): 528–537.
- [108] Chiricotto, M, Giacomelli, L, and Tomassetti, G. Dissipative scale effects in strain-gradient plasticity: the case of simple shear. *SIAM J Appl Math* 2016; 76(2): 688–704.
- [109] Djoko, JK, Ebobisse, F, McBride, AT, and Reddy, BD. A discontinuous Galerkin formulation for classical and gradient plasticity. Part 2: Algorithms and numerical analysis. *Comput Meth Appl Mech Engng* 2007; 197: 1–22.
- [110] Epstein, M. Self-driven dislocations and growth. In: Steinmann, P and Maugin, GA (eds) *Mechanics of Materials Forces (Advances in Mechanics and Mathematics, vol. 11)*, pp. 129–139. New York: Springer, 2005.
- [111] Eringen, AC. Mechanics of micromorphic continua. In: Kröner, E (ed.) *IUTAM Symposium: Mechanics of Generalized Continua*, Berlin, 1968, pp. 18–35. Berlin: Springer, 1968.
- [112] Eringen, AC. *Microcontinuum Field Theories. I. Foundations and Solids*. Berlin: Springer, 1998.
- [113] Giacomini, A, and Lussardi, L. A quasistatic evolution for a model in strain gradient plasticity. *SIAM J Math Anal* 2008; 40(3): 1201–1245.
- [114] Grandi, D and Stefanelli, U. Finite plasticity in $P^T P$. Part I: constitutive model. *Cont Mech Thermodyn* 2017; 29(1): 97–116.
- [115] Gupta, A, Steigmann, DJ, and Stölken, JS. On the evolution of plasticity and incompatibility. *Math Mech Solids* 2007; 12: 583–610.
- [116] Gupta, A, Steigmann, DJ, and Stölken, JS. Aspects of the phenomenological theory of elastic–plastic deformation. *J Elasticity* 2011; 104: 249–266.
- [117] Kratochvil, J. Finite strain theory of crystalline elastic-inelastic materials. *J Appl Phys* 1971; 42: 1104–1108.
- [118] Kraynyukova, N, Neff, P, Nesenenko, S, and Chelmiński, K. Well-posedness for dislocation based gradient visco-plasticity with isotropic hardening. *Nonlin Anal Real World Applicat* 2015; 25: 96–111.
- [119] Kröner, E. Continuum theory of defects. In: Balian, R et al. (eds.) *Les Houches, Session 35, 1980 - Physique des défauts*, pp. 215–315. New York: North-Holland, 1981.
- [120] Lee, EH. Elastic–plastic deformation at finite strain. *J Appl Mech* 1969; 36: 1–6.
- [121] Mandel, J. *Plasticité Classique et Viscoplasticité (Courses and Lectures, No. 97)*. Udine: International Center for Mechanical Sciences/Berlin: Springer, 1971.
- [122] Mielke, A. Analysis of energetic models for rate-independent materials. In: Li, T (ed.) *Proceedings of the International Congress of Mathematicians 2002*, Beijing, vol. III, pp. 817–828. Higher Education Press, 2002.
- [123] Mielke, A. Energetic formulation of multiplicative elasto-plasticity using dissipation distances. *Cont Mech Thermodyn* 2003; 15: 351–382.
- [124] Mielke, A, and Roubíček, T. Rate-independent elastoplasticity at finite strains and its numerical approximation. *Math Mod Meth Appl Sci* 2016; 26(12): 2203–2236.
- [125] Naghdi, PM. A critical review of the state of finite plasticity. *Z Angew Math Phys* 1990; 41: 315–394.
- [126] Neff, P. Remarks on invariant modelling in finite strain gradient plasticity. *Technische Mechanik* 2008; 28(1): 13–21.
- [127] Neff, P, and Ghiba, I-D. Comparison of isotropic elasto-plastic models for the plastic metric tensor $C_p = F_p^T F_p$. In: Weinberg, K and Pandolfi, A (eds.) *Innovative Numerical Approaches for Multi-Field and Multi-Scale Problems (Lecture Notes in Applied and Computational Mechanics, Vol. 81)*, pp. 161–195. New York: Springer, 2016.
- [128] Neff, P and Münch, I. Curl bounds Grad on $SO(3)$. *ESAIM Control Optim Calc Var* 2008; 14(1): 148–159.
- [129] Nye, JF. Some geometrical relations in dislocated solids. *Acta Metall* 1953; 1: 153–162.
- [130] Poh, LH, and Peerling, RHJ. The plastic rotation effect in an isotropic gradient plasticity model for applications at the meso scale. *Int J Solids Struct*. DOI: 10.1016/j.ijsolstr.2015.09.017.
- [131] Reddy, BD. The role of dissipation and defect energy in variational formulation of problems in strain-gradient plasticity. Part 1: Polycrystalline plasticity. *Cont Mech Thermodyn* 2011; 23: 527–549.
- [132] Reina, C, and Conti, S. Kinematic description of crystal plasticity in the finite kinematic framework: A micro-mechanical understanding of $F = F_e \cdot F_p$. *J Mech Phys Solids* 2014; 67: 40–61.
- [133] Sadik, S, and Yavary, A. The origins of the idea of the multiplicative decomposition of the deformation gradient. *Math Mech Solids* 2017; 22: 771–772.
- [134] Shutov, A, and Ihlemann, J. Analysis of some basic approaches to finite strain elasto-plasticity in view of reference change. *Int J Plasticity* 2014; 63: 183–197.
- [135] Sidoroff, F. Mécanique des milieux continus - Quelques réflexions sur le principe d'indifférence matérielle pour un milieu ayant un état relâché. *C R Acad Sci Paris* 1970; 271: 1026–1029.
- [136] Tsagrakis, I, and Aifantis, EC. Recent developments in gradient plasticity - Part I: Formulation and size effects. *J Eng Mater Technol* 2002; 124(3): 352–357.
- [137] Tsagrakis, I, Efremidis, G, Konstantinidis, A, and Aifantis, EC. Deformation vs. flow and wavelet-based models of gradient plasticity: Examples of axial symmetry. *Int J Plasticity* 2006; 22: 1456–1485.

Appendix

Let us first establish that

$$\operatorname{tr} \operatorname{Curl} S = 0 \quad \forall S : \mathbb{R}^3 \rightarrow \operatorname{Sym}(3) \text{ smooth tensor field.} \quad (108)$$

In fact, recalling that $(\operatorname{Curl} S)_{ij} = \sum_{kl=1}^3 \epsilon_{ikl} S_{jl,k}$ we have

$$\begin{aligned} \operatorname{tr}(\operatorname{Curl} S) &= \sum_i (\operatorname{Curl} S)_{ii} = \sum_i \sum_{kl} \epsilon_{ikl} S_{jl,k} \\ &= (S_{13,2} - S_{12,3}) + (S_{21,3} - S_{23,1}) + (S_{32,1} - S_{31,2}) = 0, \end{aligned} \quad (109)$$

because $S \in \operatorname{Sym}(3)$ and hence, $S_{13,2} = S_{31,2}$, $S_{12,3} = S_{21,3}$ and $S_{23,1} = S_{32,1}$.

The following are some further properties of Kröner's incompatibility tensor defined by

$$\operatorname{inc}(\varepsilon_p) := \operatorname{Curl}[(\operatorname{Curl} \varepsilon_p)^T]. \quad (110)$$

For the convenience of the reader, we note that

$$\operatorname{inc}(\varepsilon_p) \in \operatorname{Sym}(3) \quad \text{since} \quad \varepsilon_p \in \operatorname{Sym}(3); \quad (111)$$

$$\operatorname{inc}(\operatorname{inc}(\varepsilon_p)) \in \operatorname{Sym}(3); \quad (112)$$

$$\operatorname{tr}(\operatorname{inc}(\varepsilon_p)) = \Delta \operatorname{tr}(\varepsilon_p) - \operatorname{div}(\operatorname{Div} \varepsilon_p) = -\operatorname{div}(\operatorname{Div} \varepsilon_p) \quad \text{since} \quad \varepsilon_p \in \mathfrak{sl}(3); \quad (113)$$

$$\operatorname{tr}(\operatorname{inc}(\operatorname{inc} \varepsilon_p)) = -\Delta \operatorname{div}(\operatorname{Div} \varepsilon_p). \quad (114)$$

As (112) follows from (111), let us establish here the identities (111)-(114) for the reader's convenience. First of all, in components

$$(\operatorname{Curl} \varepsilon_p)_{ij} := \epsilon_{jkl} (\varepsilon_p)_{il,k} \quad \Leftrightarrow \quad (\operatorname{Curl} \varepsilon_p)_{ij}^T := \epsilon_{ikl} (\varepsilon_p)_{jl,k}.$$

Hence,

$$(\operatorname{inc} \varepsilon_p)_{ij} = \operatorname{Curl}[(\operatorname{Curl} \varepsilon_p)^T]_{ij} = \epsilon_{jkl} (\operatorname{Curl} \varepsilon_p)_{il,k}^T = \epsilon_{jkl} \epsilon_{imn} (\varepsilon_p)_{ln,mk}. \quad (115)$$

Now, note that $(\varepsilon_p)_{ln,mk} = (\varepsilon_p)_{nl,km}$. Therefore,

$$(\operatorname{inc} \varepsilon_p)_{ij} = \epsilon_{jkl} \epsilon_{imn} (\varepsilon_p)_{ln,mk} = \epsilon_{jmn} \epsilon_{ikl} (\varepsilon_p)_{nl,km} = \epsilon_{jmn} \epsilon_{ikl} (\varepsilon_p)_{ln,mk} = (\operatorname{inc}(\varepsilon_p))_{ji}, \quad (116)$$

which establishes (111). Now,

$$\operatorname{tr}(\operatorname{inc}(\varepsilon_p)) = (\operatorname{inc}(\varepsilon_p))_{ii} = \epsilon_{ikl} \epsilon_{imn} (\varepsilon_p)_{ln,mk}. \quad (117)$$

Using the identity

$$\epsilon_{ikl} \epsilon_{imn} = \delta_{km} \delta_{ln} - \delta_{kn} \delta_{lm} \quad (\text{see, for instance, [22, epsilon-delta identity (1.20)]}),$$

we obtain

$$\begin{aligned} \operatorname{tr}(\operatorname{inc}(\varepsilon_p)) &= \delta_{km} \delta_{ln} (\varepsilon_p)_{ln,mk} - \delta_{kn} \delta_{lm} (\varepsilon_p)_{ln,mk} = (\varepsilon_p)_{ll,mm} - (\varepsilon_p)_{lk,lk} \\ &= (\varepsilon_p)_{ll,mm} - (\varepsilon_p)_{kl,lk} = \Delta \operatorname{tr}(\varepsilon_p) - (\operatorname{Div} \varepsilon_p)_{k,k} \\ &= \Delta \operatorname{tr}(\varepsilon_p) - \operatorname{div}(\operatorname{Div} \varepsilon_p) = -\operatorname{div}(\operatorname{Div} \varepsilon_p), \end{aligned} \quad (118)$$

which establishes (113). Thus, from (113), it follows that if ε_p is a divergence-free tensor or $\operatorname{Div} \varepsilon_p$ is a divergence-free vector field, then $\operatorname{inc}(\varepsilon_p)$ becomes trace-free, that is, $\operatorname{inc}(\varepsilon_p) \in \mathfrak{sl}(3)$. Now, to establish (114), note that

$$\operatorname{Div} \operatorname{Curl} X = 0 \quad \forall X \in C^2(\Omega, \mathbb{R}^{3 \times 3}).$$

This trivially follows from our definitions of Curl and Div of a second tensor field as row-wise operations. Hence, $\operatorname{Div}(\operatorname{inc} \varepsilon_p) = 0$. Thus, using (113), we find that

$$\begin{aligned} \operatorname{tr}(\operatorname{inc}(\operatorname{inc} \varepsilon_p)) &= \Delta \operatorname{tr}(\operatorname{inc} \varepsilon_p) - \operatorname{div}(\operatorname{Div}(\operatorname{inc} \varepsilon_p)) = \Delta^2(\operatorname{tr}(\varepsilon_p) - \Delta(\operatorname{div}(\operatorname{Div} \varepsilon_p))) \\ &= -\Delta(\operatorname{div}(\operatorname{Div} \varepsilon_p)) = -\operatorname{div}(\operatorname{Div} \Delta \varepsilon_p), \end{aligned} \quad (119)$$

where $\Delta^2 = \Delta(\Delta)$ denotes the bi-Laplacian operator. Therefore, the tensor $\operatorname{inc}(\operatorname{inc} \varepsilon_p)$ is trace-free if one of the following conditions are satisfied:

- (i) ε_p is a divergence-free tensor field;
- (ii) $\text{Div } \varepsilon_p$ is a divergence-free vector field;
- (iii) $\text{div}(\text{Div } \varepsilon_p)$ is a harmonic function;
- (iv) ε_p is an harmonic tensor field;
- (v) $\Delta \varepsilon_p$ is a divergence-free tensor field;
- (vi) $\text{Div}(\Delta \varepsilon_p)$ is a divergence-free vector field.

DuEPublico

Duisburg-Essen Publications online

UNIVERSITÄT
DUISBURG
ESSEN

Offen im Denken

ub | universitäts
bibliothek

This text is made available via DuEPublico, the institutional repository of the University of Duisburg-Essen. This version may eventually differ from another version distributed by a commercial publisher.

DOI: 10.1177/1081286519845026

URN: urn:nbn:de:hbz:465-20220401-151547-8

*Ebobisse, F., & Neff, P. (2020). A fourth-order gauge-invariant gradient plasticity model for polycrystals based on Kröner's incompatibility tensor. Mathematics and Mechanics of Solids, 25(2), 129–159.
<https://doi.org/10.1177/1081286519845026>*

This publication is with permission of the rights owner freely accessible due to an Alliance licence and a national licence (funded by the DFG, German Research Foundation) respectively.

© The Author(s) 2019. All rights reserved.