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Well-posedness for the microcurl model in both single and polycrystal gradient plasticity

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ABSTRACT

We consider the recently introduced microcurl model which is a variant of strain gradient plasticity in which the curl of the plastic distortion is coupled to an additional micromorphic-type field. For both single crystal and polycrystal cases, we formulate the model and show its well-posedness in the rate-independent case provided some local hardening (isotropic or linear kinematic) is taken into account. To this end, we use the functional analytical framework developed by Han-Reddy. We also compare the model to the relaxed micromorphic model as well as to a dislocation-based gradient plasticity model.

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1. Introduction

In this paper we consider the so-called microcurl model in plasticity. The model was introduced in Forest (2013) and Cordero et al. (2013) to serve the purpose of augmenting classical plasticity with length scale effects while otherwise keeping the algorithmic structure of classical plasticity. We recall that several experimental tests on micron-sized metallic structures have shown the dependence of the mechanical response on the specimen size (see e.g. Fleck et al., 1994, 1997; Stölken and Evans, 1998). Classical theories of plasticity (see e.g. Alber, 1998; Han and Reddy, 2013; Hill, 1950) are unable to account for those size effects because they do not involve any material length scale. Various models of strain gradient plasticity have been introduced and developed in the past thirty years with the purpose to accommodate the experimentally observed size effects in material behaviour in small scales. The size effects are captured through the introduction of plastic strain gradient (or its higher derivatives) and sometimes together with higher order stress tensors in the constitutive equations (see e.g. Aifantis, 1984; Aifantis, 1987, 2003; Fleck and Hutchinson, 2001; Gurtin, 2004; Gudmundson, 2004; Gurtin and Anand, 2005, 2009; Gurtin and Reddy, 2014; Fleck and Willis, 2009a, 2009b; Menzel and Steinmann, 1998; Menzel and Steinmann, 2000; Mühlhaus and Aifantis, 1991; Reddy, 2011a; Svendsen et al., 2009 and also the recent contributions in Anand et al., 2015;

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Chiricotto et al., 2016; Chang et al., 2012; El-Naaman et al., 2016; Le and Günther, 2014; Wulfinghof and Böhlke, 2015; Wulfinghof et al., 2013). Models of strain gradient plasticity lead to the flow law involving nonlocal terms.

The idea in the microcurl model is simple and straight-forward: the in general non-symmetric plastic distortion p (single crystal plasticity and polycrystal plasticity with plastic spin) with its local in space evolution is energetically coupled to a micromorphic-type additional non-symmetric tensorial variable χ_p via a penalty-like term $\frac{1}{2}\mu\, H_\chi \|p-\chi_p\|^2$. The tensor field χ_p is generally assumed to be incompatible i.e., it may not derive from a vector field. The total energy in the model is then augmented by a quadratic contribution acting on the Curl of χ_p. The new variable χ_p is now determined by free-variation of the energy w.r.t. the displacement field u and the micromorphic field χ_p together with corresponding tangential boundary conditions for χ_p. This generates the usual equilibrium equation on the one hand and what we will call a micro-balance equation for χ_p on the other hand.

In the penalty limit $H_\chi \to \infty$, when one expects $p=\chi_p$, the variable Curl χ_p is then interpreted to be the dislocation density tensor Curl p. The advantage of such a formulation is clear: there is no need for an extended thermodynamic setting, since χ_p is not directly taking part in the dissipation. Constitutive laws including dissipative contributions of the microdeformation and microcurl can be proposed, as done in Forest and Sievert (2006) in the general micromorphic case, but they will require additional material parameters whose identification necessitates material specific physical considerations. Thus, also no higher order boundary conditions at interfaces between elastic and plastic parts need be discussed. The resulting model can therefore be described as a *pseudo-regularized strain gradient model*.

The microdeformation variable χ_p has at least two different interpretations. First, it can be regarded as a mathematical auxiliary variable used to replace the higher order partial differential equations arising in strain gradient plasticity by a system of two sets of second order partial differential equations for the displacement and microdeformation. This method has computational merits for the implementation of strain gradient plasticity models in finite element codes, see Anand et al. (2012). In that case, H_χ is regarded as a mere penalty parameter and should be large enough to enforce the constraint $p=\chi_p$. In contrast, the microdeformation variable χ_p can also be viewed as a constitutive variable with physical interpretation, for instance based on statistical mechanics, p representing the average plastic distortion over the material volume element and χ_p being related to the variance of plastic deformation inside this volume. This interpretation is similar to the microconcentration variable introduced in Ubachs et al. (2004) and Forest et al. (2014) to solve Cahn–Hilliard equations. In this context, H_χ must be regarded as a true material higher order modulus to be identified from suitable experimental results. Compared to standard strain gradient plasticity, the microcurl model therefore possesses one additional parameter, H_χ, which allows for better description of physical results, as suggested in Cordero et al. (2010). An interpretation of the microdeformation χ_p was recently proposed in the case of polycrystalline plasticity and damage in Poh (2013) and Poh and Peerlings (2016) where it is related to the grain to grain heterogeneity of plastic deformation.

Another computational advantage of the microcurl single crystal plasticity model is that the number of independent degrees of freedom (9 tensor components of χ_p, or 8 in the case of incompressible microplasticity) is independent of the crystallographic structure of the material and of the number of slip systems. This is in contrast to strain gradient plasticity models involving the directional gradient of the slip variables (Gurtin, 2002), which require as many degrees of freedom as slip systems (12 at least in FCC crystals, up to 48 in BCC crystals!). A comparison and discussion of models based on the full dislocation density tensors with models involving densities of geometrically necessary dislocations can be found in Mesarovic et al. (2015). A variant to the microcurl model for single crystal plasticity was proposed in Bayerschen and Böhlke (2016) where the micromorphic variable is rather a scalar which is coupled with an equivalent plastic strain measure, defined as the average of the plastic slips along all the slip planes.

In this paper we will consider the microcurl model in two variants. First, in its original form as a computational approach towards single crystal strain gradient plasticity. We formulate the governing system and show its well-posedness in the rate-independent case. The natural solution space for the micro-variable χ_p is the Sobolev-like space $H(\mathrm{Curl})$.

Second, we extend the approach formally to polycrystalline plasticity in which the plastic variable $\varepsilon_p := \mathrm{sym}\, p$ (the plastic strain) is assumed to be symmetric. In this case we still allow for a non-symmetric micro-variable χ_p which is now coupled to the plastic variable only via its symmetric part by $\frac{1}{2}\mu\, H_\chi \|\mathrm{sym}(p-\chi_p)\|^2$. This represents an alternative to recently proposed strain gradient plasticity models involving a plastic spin tensor for polycrystals (Gurtin, 2004; Bardella and Panteghini, 2015; Poh and Peerlings, 2016). Again, we show the well-posedness of the formulation. Here, we need recently introduced coercive inequalities generalizing Korn's inequality to incompatible tensor fields (Bauer et al., 2014, 2016; Neff et al., 2011, 2012a, 2012b, 2014b).

The mathematical analysis (with results of existence and uniqueness) for both variants (single crystal and polycrystalline) is obtained through the machinery developped by Han and Reddy (2013), Theorems 6.15 and 6.19 for classical plasticity and recently extended to models of gradient plasticity in Djoko et al. (2007a), Neff et al. (2009a), Ebobisse and Neff (2010), Ebobisse et al. (2016a) and Ebobisse et al. (2016b). In this approach, the model through the primal form of the flow rule is weakly formulated as a variational inequality and the key issue for its well-posedness is the study of the coercivity of the bilinear form involved on a suitable closed convex subset of some Hilbert space. Let us mention that, other mathematical and computational results for higher order models related to gradient plasticity theories were obtained in the past years (see e.g. Bargmann et al., 2014; Djoko et al., 2007a, 2007b; Ebobisse et al., 2008; Kraynyukova et al., 2015; Neff, 2006, 2008; Neff and Reddy, 2008; Neff et al., 2009b; Nesenenko and Neff, 2012; Nesenenko and Neff, 2013; Nguyen, 2011; Reddy, 2011b; Reddy et al., 2014).

The polycrystalline variant of the microcurl model bears some superficial resemblence with the recently introduced relaxed micromorphic models (Neff et al., 2014a, 2015). For purpose of clarification, we present the relaxed micromorphic model and clearly point out the differences. In order to put the microcurl modelling framework further on display we finish this introduction with another dislocation based strain gradient plasticity model with plastic spin (Ebobisse and Neff, 2010; Ebobisse et al., 2016a; Ebobisse et al., 2016b), see Table 1.

Here, the microcurl-type regularization would be obtained by considering the microcurl energy

$$\frac{1}{2}\langle \mathbb{C}_{\text{iso}}\varepsilon_e, \varepsilon_e\rangle + \frac{1}{2}\mu\, H_\chi \|p-\chi_p\|^2 + \frac{1}{2}\mu\, k_1 \|\text{sym}\, p\|^2 + \frac{1}{2}\mu\, L_c^2\, \|\text{Curl}\, \chi_p\|^2 \tag{1.1}$$

and for $H_\chi \to \infty$ we would recover the model from Table 1.

The polycrystalline microcurl variant which we introduce in this paper is, however, based on the energy

$$\frac{1}{2}\langle \mathbb{C}_{\text{iso}}\varepsilon_e, \varepsilon_e\rangle + \frac{1}{2}\mu\, H_\chi \|\text{sym}(p-\chi_p)\|^2 + \frac{1}{2}\mu\, k_1 \|\text{sym}\, p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\text{Curl}\, \chi_p\|^2. \tag{1.2}$$

This ansatz seems to be appropriate for polycrystalline plasticity without plastic spin.

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 the elastoplastic body in its undeformed configuration. Let Γ_{D} be a smooth subset of $\partial\Omega$ with non-vanishing 2-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 $|a|^2_{\mathbb{R}^3} = \langle a, a\rangle_{\mathbb{R}^3}$. 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 $\text{tr}(A) = \langle A, \mathbb{1}\rangle$. The set $\mathfrak{so}(3) := \{X \in \mathbb{R}^{3\times 3} \,|\, X^T = -X\}$ is the Lie-Algebra of skew-symmetric tensors. We let $\text{Sym}(3) := \{X \in \mathbb{R}^{3\times 3} \,|\, X^T = X\}$ denote the vector space of symmetric tensors and $\mathfrak{sl}(3) := \{X \in \mathbb{R}^{3\times 3} \,|\, \text{tr}\,(X) = 0\}$ 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., $\overline{A} \in \mathfrak{so}(3)$ for the function $A : \mathbb{R}^3 \to \mathfrak{so}(3)$ which is constant with constant value $\overline{A}$.

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

- u is the displacement of the macroscopic material points;
- 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 a state-variable, while the rate $\dot{p}$ is an infinitesimal state variable in some suitable sense;
- $e = \nabla u - p$ is the infinitesimal elastic distortion which is in general a non-symmetric second order tensor and is an infinitesimal state-variable;
- $\varepsilon_p = \text{sym}\, p$ is the symmetric infinitesimal plastic strain tensor, which is trace free, $\varepsilon_p \in \mathfrak{sl}(3)$; ε_p is not a state-variable; the rate $\dot{\varepsilon}_p$ is an infinitesimal state-variable;
- $\varepsilon_e = \text{sym}\nabla u - \varepsilon_p$ is the symmetric infinitesimal elastic strain tensor and is an infinitesimal state-variable;

Table 1
The polycrystalline plasticity model with linear kinematic hardening and plastic spin studied in Ebobisse et al. (2016a).

Additive split of distortion:	$\nabla u = e + p, \quad \varepsilon_e := \text{sym}\, e, \quad \varepsilon_p := \text{sym}\, p$
Equilibrium:	$\text{Div}\,\sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}}\varepsilon_e$
Free energy:	$\frac{1}{2}\langle \mathbb{C}_{\text{iso}}\varepsilon_e, \varepsilon_e\rangle + \frac{1}{2}\mu\, k_1 \|\varepsilon_p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\text{Curl}\, p\|^2$
Yield condition:	$\phi(\Sigma_E) := \|\text{dev}\, \Sigma_E\| - \sigma_0 \le 0$
where	$\Sigma_E := \sigma + \Sigma^{\text{lin}}_{\text{curl}} + \Sigma^{\text{lin}}_{\text{kin}}$,
	$\Sigma^{\text{lin}}_{\text{curl}} := -\mu\, L_c^2\, \text{Curl Curl}\, p, \quad \Sigma^{\text{lin}}_{\text{kin}} := -\mu\, k_1\, \varepsilon_p$
Dissipation inequality:	$\int_\Omega \langle \Sigma_E, \dot{p}\rangle dx \ge 0$
Dissipation function:	$\mathscr{D}(q) := \sigma_0 \|q\|$
Flow rule in primal form:	$\Sigma_E \in \partial\mathscr{D}(\dot{p})$
Flow rule in dual form:	$\dot{p} = \lambda \frac{\text{dev}\, \Sigma_E}{\|\text{dev}\, \Sigma_E\|}, \quad \lambda = \|\dot{p}\|$
KKT conditions:	$\lambda \ge 0, \quad \phi(\Sigma_E) \le 0, \quad \lambda\phi(\Sigma_E) = 0$
Boundary conditions for p:	$p \times n = 0$ on Γ_{D}, $(\text{Curl}\, p) \times n = 0$ on $\partial\Omega \setminus \Gamma_{\text{D}}$
Function space for p:	$p(t, \cdot) \in \text{H(Curl;}\ \Omega,\ \mathbb{R}^{3\times 3})$

- $\chi_p \in \mathbb{R}^{3\times 3}$ is the non-symmetric infinitesimal micro-distortion with $\operatorname{sym}\chi_p$ being the symmetric micro-strain;
- σ is the Cauchy stress tensor which is a symmetric second order tensor and is an infinitesimal state-variable;
- σ_0 is the initial yield stress for plastic variables p or $\varepsilon_p := \operatorname{sym} p$ and is an infinitesimal state-variable;
- f is the body force;
- $\operatorname{Curl} p = \alpha$ is the dislocation density tensor satisfying the so-called Bianchi identities $\operatorname{Div}\alpha = 0$ and is an infinitesimal state-variable;
- $\eta_p = \int_0^t \|\dot{e}_p\|\, ds$ is the accumulated equivalent plastic strain and is an infinitesimal state-variable;
- γ^α is the slip in the α-th slip system in single crystal plasticity while l^α is the slip direction and ν^α is the normal vector to the slip plane with $\alpha = 1, \dots, n_{\text{slip}}$. Hence, $p = \sum_\alpha \gamma^\alpha l^\alpha \otimes \nu^\alpha$.

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

$$\mathbb{C}_{\text{iso}} \operatorname{sym} X = 2\mu \operatorname{dev}\operatorname{sym} X + \kappa \operatorname{tr}(X)\mathbb{1} = 2\mu \operatorname{sym} X + \lambda \operatorname{tr}(X)\mathbb{1} \tag{2.1}$$

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

$$\mu > 0 \quad \text{and} \quad 3\lambda + 2\mu > 0, \tag{2.2}$$

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

$$\forall X \in \mathbb{R}^{3\times 3}: \quad \langle \operatorname{sym} X, \mathbb{C}_{\text{iso}} \operatorname{sym} X\rangle \geq m_0 \|\operatorname{sym} X\|^2. \tag{2.3}$$

The space of square integrable functions is $L^2(\Omega)$, while the Sobolev spaces used in this paper are:

$$\begin{aligned} \mathrm{H}^1(\Omega) &= \{u \in L^2(\Omega) \,|\, \operatorname{grad} u \in L^2(\Omega)\}, \quad \operatorname{grad} = \nabla, \\ &\|u\|^2_{H^1(\Omega)} = \|u\|^2_{L^2(\Omega)} + \|\operatorname{grad} u\|^2_{L^2(\Omega)}, \quad \forall u \in \mathrm{H}^1(\Omega), \\ \mathrm{H}(\operatorname{curl};\Omega) &= \{v \in L^2(\Omega) \mid \operatorname{curl} v \in L^2(\Omega)\}, \quad \operatorname{curl} = \nabla\times, \\ &\|v\|^2_{\mathrm{H}(\operatorname{curl};\Omega)} = \|v\|^2_{L^2(\Omega)} + \|\operatorname{curl} v\|^2_{L^2(\Omega)}, \quad \forall v \in \mathrm{H}(\operatorname{curl};\ \Omega). \end{aligned} \tag{2.4}$$

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 $\operatorname{Curl} X$ in Neff et al. (2009a) and Svendsen (2002):

$$\operatorname{Curl} X = \begin{pmatrix} \operatorname{curl} X^1 \,--\\ \operatorname{curl} X^2 \,--\\ \operatorname{curl} X^3 \,-- \end{pmatrix} \in \mathbb{R}^{3\times 3}, \tag{2.5}$$

for which $\operatorname{Curl}\ \nabla v = 0$ for every $v \in C^2(\Omega,\ \mathbb{R}^3)$. Notice that the definition of $\operatorname{Curl} X$ above is such that $(\operatorname{Curl} X)^T a = \operatorname{curl}\ (X^T a)$ for every $a \in \mathbb{R}^3$ and this clearly corresponds to the transpose of the Curl of a tensor as defined in Gurtin and Anand (2005) and Gurtin et al. (2010).

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

$$\begin{aligned} \mathrm{H}(\operatorname{Curl};\ \Omega,\ \mathbb{R}^{3\times 3}) &= \{X \in L^2(\Omega,\ \mathbb{R}^{3\times 3}) \mid \operatorname{Curl} X \in L^2(\Omega,\ \mathbb{R}^{3\times 3})\}, \\ \|X\|^2_{\mathrm{H}(\operatorname{Curl};\Omega)} &= \|X\|^2_{L^2(\Omega)} + \|\operatorname{Curl} X\|^2_{L^2(\Omega)}, \quad \forall X \in \mathrm{H}(\operatorname{Curl};\ \Omega,\ \mathbb{R}^{3\times 3}), \\ \mathrm{H}(\operatorname{Curl};\ \Omega,\ \mathbb{E}) &= \{X : \Omega \to \mathbb{E} \,|\, X \in \mathrm{H}(\operatorname{Curl};\ \Omega,\ \mathbb{R}^{3\times 3})\}, \end{aligned} \tag{2.6}$$

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

We also consider the space

$$\mathrm{H}_0(\operatorname{Curl};\ \Omega,\ \Gamma_D, \mathbb{R}^{3\times 3}) \tag{2.7}$$

as the completion in the norm in (2.6) of the space $\{X \in C^\infty(\Omega, \mathbb{R}^{3\times 3}) \mid X \times n|_{\Gamma_D} = 0\}$.

Therefore, this space generalizes the tangential Dirichlet boundary condition

$$X \times n\big|_{\Gamma_D} = 0$$

to be satisfied by the plastic micro-distortion χ_p. The space

$$\mathrm{H}_0(\operatorname{Curl};\Omega,\Gamma_D,\mathbb{E})$$

is defined as in (2.6).

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

$$\mathrm{Div}\, X = \begin{pmatrix} \mathrm{div}\, X_1 \\ \mathrm{div}\, X_2 \\ \mathrm{div}\, X_3 \end{pmatrix}. \tag{2.8}$$

3. The microcurl model in single crystal gradient plasticity

3.1. Kinematics

Single-crystal plasticity is based on the assumption that the plastic deformation happens through crystallograpic shearing which represents the dislocation motion along specific slip systems, each being characterized by a plane with unit normal ν^α and slip direction l^α on that plane, and slips $\gamma^\alpha (\alpha = 1, \dots, n_{\mathrm{slip}})$. The flow rule for the plastic distortion p is written at the slip system level by means of the orientation tensor m^α defined as

$$m^\alpha := l^\alpha \otimes \nu^\alpha. \tag{3.1}$$

Under these conditions the plastic distortion p takes the form

$$p = \sum_{\alpha=1}^{n_{\mathrm{slip}}} \gamma^\alpha m^\alpha \tag{3.2}$$

so that the plastic strain $\varepsilon_p = \mathrm{sym}\, p$ is

$$\varepsilon_p = \sum_{\alpha=1}^{n_{\mathrm{slip}}} \gamma^\alpha \mathrm{sym}(m^\alpha) = \frac{1}{2} \sum_{\alpha=1}^{n_{\mathrm{slip}}} \gamma^\alpha (l^\alpha \otimes \nu^\alpha + \nu^\alpha \otimes l^\alpha) \tag{3.3}$$

and $\mathrm{tr}(p) = 0$ since $l^\alpha \perp \nu^\alpha$.

For the slips $\gamma^\alpha (\alpha = 1, \dots, n_{\mathrm{slip}})$ we set

$$\underline{\gamma} := (\gamma^1, \dots, \gamma^{n_{\mathrm{slip}}}).$$

Therefore, we get from (3.3) that

$$p = \overline{m}\, \underline{\gamma}, \tag{3.4}$$

where $\overline{m}$ is the third order tensor[1] defined as

$$\overline{m}_{ij\alpha} := m^\alpha_{ij} = l^\alpha_i \nu^\alpha_j \quad \text{for} \quad i,j = 1,2,3 \text{ and } \alpha = 1, \dots, n_{\mathrm{slip}}. \tag{3.5}$$

Let $\underline{\eta} := (\eta^1, \dots, \eta^{n_{\mathrm{slip}}})$ with η^α being a hardening variable in the α-th slip system.

3.2. The case with isotropic hardening

The starting point is the total energy

$$\mathscr{E}(u, \underline{\gamma}, \chi_p, \underline{\eta}) := \int_\Omega \Big[\Psi(\nabla u, \underline{\gamma}, \chi_p, \mathrm{Curl}\, \chi_p, \underline{\eta}) - \langle f, u \rangle \Big] dx \tag{3.6}$$

where the free-energy density Ψ is given in the additively separated form

[1] The terminology "tensor" used here is just intended as "matrix" since $\overline{m}$ does not fulfill the rules of change of orthogonal bases for the last index and therefore is not a tensor in the usual sense.

$$\Psi(\nabla u, \underline{\gamma}, \chi_p, \mathrm{Curl}\,\chi_p, \underline{\eta}) := \underbrace{\Psi_e^{\mathrm{lin}}(\varepsilon_e)}_{\text{elastic energy}} + \underbrace{\Psi_{\mathrm{micro}}^{\mathrm{lin}}(p, \chi_p)}_{\text{micro energy}} + \underbrace{\Psi_{\mathrm{curl}}^{\mathrm{lin}}(\mathrm{Curl}\chi_p)}_{\text{defect-like energy (GND)}} + \underbrace{\Psi_{\mathrm{iso}}(\underline{\eta})}_{\text{hardening energy (SSD)}}, \tag{3.7}$$

where

$$\begin{aligned} \Psi_e^{\mathrm{lin}}(\varepsilon_e) &:= \frac{1}{2}\langle \varepsilon_e, \mathbb{C}_{\mathrm{iso}}\varepsilon_e\rangle = \frac{1}{2}\langle \mathrm{sym}(\nabla u - p), \mathbb{C}_{\mathrm{iso}}\mathrm{sym}(\nabla u - p)\rangle, \\ \Psi_{\mathrm{micro}}^{\mathrm{lin}}(p, \chi_p) &:= \frac{1}{2}\mu\, H_\chi \|p - \chi_p\|^2, \quad \Psi_{\mathrm{curl}}^{\mathrm{lin}}(\mathrm{Curl}\,\chi_p) := \frac{1}{2}\mu\, L_c^2 \|\mathrm{Curl}\,\chi_p\|^2, \\ \Psi_{\mathrm{iso}}(\underline{\eta}) &:= \frac{1}{2}\mu\, k_2 \|\underline{\eta}\|^2 = \frac{1}{2}\mu\, k_2 \sum_\alpha |\eta^\alpha|^2. \end{aligned} \tag{3.8}$$

Here, $L_c \geq 0$ is an energetic length scale which characterizes the contribution of the defect-like energy density to the system, H_χ is a positive nondimensional penalty constant, k_2 is a positive nondimensional isotropic hardening constant.

The starting point for the derivation of the equations and inequalities describing the plasticity model is the two-field minimization formulation

$$\mathscr{E}(u, \underline{\gamma}, \chi_p, \underline{\eta}) \quad \rightarrow \quad \text{min. w.r.t. } (u, \chi_p). \tag{3.9}$$

The first variations of the total energy w.r.t. to the variables u and χ_p lead to the balance equations in the next section.

3.2.1. The balance equations

The conventional macroscopic force balance leads to the equation of equilibrium

$$\mathrm{div}\,\sigma + f = 0 \tag{3.10}$$

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

An additional microscopic balance equation is obtained as follows. Precisely, the first variation of the total energy w.r.t. χ_p gives for every $\delta\chi_p \in C^\infty(\Omega, \mathbb{R}^{3\times 3})$,

$$\begin{aligned} 0 &= \frac{d}{dt}\mathscr{E}(u, p, \chi_p + t\delta\chi_p, \underline{\eta})\Big|_{t=0} \\ &= \int_\Omega \Big[\mu\, H_\chi \langle \chi_p - p, \delta\chi_p\rangle + \mu\, L_c^2 \langle \mathrm{Curl}\,\chi_p, \mathrm{Curl}\,\delta\chi_p\rangle\Big] dx \\ &= \int_\Omega \Big[\mu\, H_\chi\, \langle \chi_p - p, \delta\chi_p\rangle + \mu\, L_c^2 \langle \mathrm{Curl}\,\mathrm{Curl}\,\chi_p, \delta\chi_p\rangle + \sum_{i=1}^3 \mathrm{div}\big(\mu L_c^2\, \delta\chi_p^i \times (\mathrm{Curl}\,\chi_p)^i\big)\Big] dx \\ &= \int_\Omega \langle \mu\, H_\chi\, (\chi_p - p) + \mu\, L_c^2 \mathrm{Curl}\,\mathrm{Curl}\,\chi_p, \delta\chi_p\rangle \mathrm{dx} + \sum_{i=1}^3 \int_{\partial\Omega} \mu L_c^2 \langle \delta\chi_p^i \times (\mathrm{Curl}\,\chi_p)^i, n\rangle da, \end{aligned} \tag{3.11}$$

which on the one hand gives from the choice $\delta\chi_p \in C_c^\infty(\Omega, \mathbb{R}^{3\times 3})$ the micro-balance in strong formulation[2]

$$\mu\, L_c^2\, \mathrm{Curl}\,\mathrm{Curl}\,\chi_p = -\mu\, H_\chi(\chi_p - p). \tag{3.12}$$

One the other hand we get

$$\sum_{i=1}^3 \int_{\partial\Omega} \mu L_c^2 \langle \delta\chi_p^i \times (\mathrm{Curl}\,\chi_p)^i, n\rangle da = 0 \quad \forall\, \delta\chi_p \in C^\infty(\Omega, \mathbb{R}^{3\times 3}) \tag{3.13}$$

which is satisfied if we choose certain homogeneous boundary conditions on the micro-distortion χ_p. Following Gurtin (2004) and also Gurtin and Needleman (2005) we choose the simple boundary condition

[2] Here, we have assumed uniform material constants for simplicity.

$$\chi_p \times n|_{\Gamma_D} = 0 \quad \text{and} \quad (\text{Curl}\,\chi_p) \times n|_{\partial\Omega\setminus\Gamma_D} = 0 \tag{3.14}$$

which in the case of models in strain gradient plasticity, where χ_p is replaced by p or ε_p simply implies that there is no flow of the plastic distortion or plastic strain across the piece Γ_D of the boundary $\partial\Omega$.

3.2.2. The derivation of the dissipation inequality

The local free-energy imbalance states that

$$\dot{\Psi} - \langle \sigma, \dot{\varepsilon}_e \rangle - \langle \sigma, \dot{p} \rangle \leq 0. \tag{3.15}$$

Now we expand the first term, substitute (3.7)–(3.8) and get

$$\langle \mathbb{C}_{\text{iso}}\, \varepsilon_e - \sigma, \dot{\varepsilon}_e \rangle - \sum_\alpha \langle \sigma, m^\alpha \rangle \dot{\gamma}^\alpha + \sum_\alpha \frac{\partial \Psi^{\text{lin}}_{\text{micro}}}{\partial \gamma^\alpha} \dot{\gamma}^\alpha + \sum_\alpha \frac{\partial \Psi_{\text{iso}}}{\partial \eta^\alpha} \dot{\eta}^\alpha \leq 0. \tag{3.16}$$

That is

$$\langle \mathbb{C}_{\text{iso}}\, \varepsilon_e - \sigma, \dot{\varepsilon}_e \rangle - \sum_\alpha \langle \sigma, m^\alpha \rangle \dot{\gamma}^\alpha - \sum_\alpha \mu\, H_\chi \langle \chi_p - p, m^\alpha \rangle \dot{\gamma}^\alpha + \mu\, k_2 \sum_\alpha \eta^\alpha \dot{\eta}^\alpha \leq 0. \tag{3.17}$$

Therefore we obtain

$$0 \leq -\langle \mathbb{C}_{\text{iso}}\, \varepsilon_e - \sigma, \dot{\varepsilon}_e \rangle + \sum_\alpha [(\tau^\alpha + s^\alpha)\dot{\gamma}^\alpha + g^\alpha \dot{\eta}^\alpha] = -\langle \mathbb{C}_{\text{iso}}\, \varepsilon_e - \sigma, \dot{\varepsilon}_e \rangle + \sum_\alpha [\tau^\alpha_{\text{E}} \dot{\gamma}^\alpha + g^\alpha \dot{\eta}^\alpha], \tag{3.18}$$

where we set

$$\tau^\alpha := \langle \sigma, m^\alpha \rangle \quad (\text{resolved shear stress for the } \alpha - \text{th slip system}), \tag{3.19}$$

$$s^\alpha := \mu\, H_\chi \langle \chi_p - p, m^\alpha \rangle = -\mu\, L_c^2 \langle \text{Curl Curl}\, \chi_p, m^\alpha \rangle, \tag{3.20}$$

$$g^\alpha := -\mu\, k_2\, \eta^\alpha \quad (\text{thermodynamic force power} - \text{conjugate to } \dot{\eta}^\alpha), \tag{3.21}$$

$$\tau^\alpha_{\text{E}} := \tau^\alpha + s^\alpha = \langle \Sigma_E, m^\alpha \rangle, \tag{3.22}$$

with Σ_E being the non-symmetric Eshelby-type stress tensor defined by

$$\Sigma_E := \sigma + \mu\, H_\chi (\chi_p - p) = \sigma - \mu\, L_c^2\, \text{Curl Curl}\, \chi_p. \tag{3.23}$$

Since the inequality (3.18) must be satisfied for whatever elastic-plastic deformation mechanism, including purely elastic ones (for which $\dot{\gamma}^\alpha = 0$, $\dot{\eta}^\alpha = 0$), Equation (3.18) implies the usual infinitesimal elastic stress-strain relation

$$\begin{aligned} \sigma = \mathbb{C}_{\text{iso}}\, \varepsilon_e \quad &= 2\mu\, \text{sym}(\nabla u - p) + \lambda\, \text{tr}(\nabla u - p)\mathbb{1} \\ &= 2\mu\, (\text{sym}(\nabla u) - \varepsilon_p) + \lambda\, \text{tr}(\nabla u)\mathbb{1} \end{aligned} \tag{3.24}$$

and the local reduced dissipation inequality

$$\sum_\alpha [\tau^\alpha_E\, \dot{\gamma}^\alpha + g^\alpha\, \dot{\eta}^\alpha] \geq 0 \tag{3.25}$$

which can also be written in compact form as

$$\sum_\alpha \langle \Sigma^\alpha_p, \dot{\Gamma}^\alpha_p \rangle \geq 0, \tag{3.26}$$

where we define

$$\Sigma^\alpha_p := (\tau^\alpha_E, g^\alpha) \quad \text{and} \quad \Gamma^\alpha_p := (\gamma^\alpha, \eta^\alpha). \tag{3.27}$$

3.2.3. The flow rule

We consider a yield function on the α-th slip system defined by

$$\phi(\Sigma_p^\alpha) := |\tau_{\mathrm{E}}^\alpha| + g^\alpha - \sigma_0 \quad \text{for} \quad \Sigma_p^\alpha = (\tau_{\mathrm{E}}^\alpha, g^\alpha)\,. \tag{3.28}$$

Here, σ_0 is the yield stress of the material, that we assume to be constant on all slip systems and therefore, $\sigma_{\mathrm{y}}^\alpha := \sigma_0 - g^\alpha$ represents the current yield stress for the α-th slip system.[3] So the set of admissible generalized stresses for the α-th slip system is defined as

$$\mathscr{K}^\alpha := \Big\{\Sigma_p^\alpha = (\tau_{\mathrm{E}}^\alpha, g^\alpha) \;\big|\; \phi(\Sigma_p^\alpha) \le 0,\;\; g^\alpha \le 0\Big\}, \tag{3.29}$$

with its interior $\mathrm{Int}(\mathscr{K}^\alpha)$ and its boundary $\partial\mathscr{K}^\alpha$ being the generalized elastic region and the yield surface for the α-th slip system, respectively.

The principle of maximum dissipation[4] associated with the α-th slip system gives us the normality law

$$\dot\Gamma_p^\alpha \in N_{\mathscr{K}^\alpha}(\Sigma_p^\alpha), \tag{3.30}$$

where $N_{\mathscr{K}^\alpha}(\Sigma_p^\alpha)$ denotes the normal cone to $\mathscr{K}^\alpha$ at Σ_p^α. That is, $\dot\Gamma_p^\alpha$ satisfies

$$\big\langle \overline{\Sigma}^\alpha - \Sigma_p^\alpha, \dot\Gamma_p^\alpha\big\rangle \le 0 \quad \text{for all } \overline{\Sigma}^\alpha \in \mathscr{K}^\alpha\,. \tag{3.31}$$

Notice that $N_{\mathscr{K}^\alpha} = \partial\chi_{\mathscr{K}^\alpha}$, where $\chi_{\mathscr{K}^\alpha}$ denotes the indicator function of the set $\mathscr{K}^\alpha$ and $\partial\chi_{\mathscr{K}^\alpha}$ denotes the subdifferential of the function $\chi_{\mathscr{K}^\alpha}$.

Whenever the yield surface $\partial\mathscr{K}^\alpha$ is smooth at Σ_p^α then

$$\dot\Gamma_p^\alpha \in N_{\mathscr{K}^\alpha}(\Sigma_p^\alpha) \quad \Rightarrow \quad \exists\,\lambda^\alpha \text{ such that } \dot\gamma^\alpha = \lambda^\alpha \frac{\tau_{\mathrm{E}}^\alpha}{|\tau_{\mathrm{E}}^\alpha|} \quad \text{and} \quad \dot\eta^\alpha = \lambda^\alpha = |\dot\gamma^\alpha|$$

with the Karush-Kuhn Tucker conditions: $\lambda^\alpha \ge 0$, $\phi(\Sigma_p^\alpha) \le 0$ and $\lambda^\alpha\phi(\Sigma_p^\alpha) = 0$.

Using convex analysis (Legendre-transformation) we find that

$$\underbrace{\dot\Gamma_p^\alpha \in \partial\chi_{K^\alpha}(\Sigma_p^\alpha)}_{\text{flow rule in its dual formulation for the } \alpha\text{-th slip system}} \tag{3.32}$$

$$\Updownarrow$$

$$\underbrace{\Sigma_p^\alpha \in \partial\chi^*_{K^\alpha}(\dot\Gamma_p^\alpha)}_{\text{flow rule in its primal formulation for the } \alpha\text{-th slip system}} \tag{3.33}$$

where $\chi^*_{\mathscr{K}^\alpha}$ is the Fenchel-Legendre dual of the function $\chi_{\mathscr{K}^\alpha}$ denoted in this context by $\mathscr{D}^\alpha_{\mathrm{iso}}$, the one-homogeneous dissipation function for the α-th slip system. That is, for every $\Gamma^\alpha = (q^\alpha, \beta^\alpha)$,

$$\begin{aligned}\mathscr{D}^\alpha_{\mathrm{iso}}(\Gamma^\alpha) &= \sup\Big\{\langle \Sigma_p^\alpha, \Gamma^\alpha\rangle \;\Big|\; \Sigma_p^\alpha \in \mathscr{K}^\alpha\Big\}\\ &= \sup\big\{\tau_E^\alpha\, q^\alpha + g^\alpha\beta^\alpha \big|\; \phi(\Sigma_E^\alpha, g^\alpha) \le 0,\;\; g^\alpha \le 0\big\}\\ &= \begin{cases} \sigma_0|q^\alpha| & \text{if } |q^\alpha| \le \beta^\alpha,\\ \infty & \text{otherwise.}\end{cases}\end{aligned} \tag{3.34}$$

We get from the definition of the subdifferential $(\Sigma_p^\alpha \in \partial\chi^*_{\mathscr{K}^\alpha}(\dot\Gamma_p^\alpha))$ that

$$\mathscr{D}^\alpha_{\mathrm{iso}}(\Gamma^\alpha) \ge \mathscr{D}^\alpha_{\mathrm{iso}}(\dot\Gamma_p^\alpha) + \langle \Sigma_p^\alpha, \Gamma^\alpha - \dot\Gamma_p^\alpha\rangle \quad \text{for any } \Gamma^\alpha. \tag{3.35}$$

That is,

[3] Note that, for the sake of simplicity, the presented isotropic hardening rule g^α does not involve latent hardening and the associated interaction matrix, see Franciosi and Zaoui (1991) for a discussion on uniqueness in the presence of latent hardening.

[4] The principle of maximum dissipation (PMD) is shown to be closely related to the so-called minimum principle for the dissipation potential (MPDP) (Hackl and Fischer, 2008; Hackl, 1997; Ortiz and Repetto, 1999), which states that the rate of the internal variables is the minimizer of a functional consisting of the sum of the rate of the free energy and the dissipation function with respect to appropriate boundary conditions. Notice that, as pointed out in Ebobisse et al. (2016a), both PMD and MPDP are not physical principles but thermodynamically consistent selection rules which turn out to be convenient if no other information is available or if existing flow rules are to be extended to a more general situation.

$$\mathscr{D}^{\alpha}_{\mathrm{iso}}(q^{\alpha},\beta^{\alpha}) \geq \mathscr{D}^{\alpha}_{\mathrm{iso}}(\dot{\gamma}^{\alpha},\dot{\eta}^{\alpha}) + \tau^{\alpha}_{\mathrm{E}}(q^{\alpha}-\dot{\gamma}^{\alpha}) + g^{\alpha}(\beta^{\alpha}-\dot{\eta}^{\alpha}) \quad \text{for any } (q^{\alpha},\beta^{\alpha}). \tag{3.36}$$

In the next sections, we present a complete mathematical analysis of the model including both strong and weak formulations as well as a corresponding existence result.

3.2.4. Strong formulation of the model

To summarize, we have obtained the following strong formulation for the microcurl model in the single crystal infinitesimal gradient plasticity case with isotropic hardening. Given $f \in \mathrm{H}^1(0,T;L^2(\Omega,\mathbb{R}^3))$, the goal is to find:

(i) the displacement $u \in \mathrm{H}^1(0,T;H^1_0(\Omega,\Gamma_{\mathrm{D}},\mathbb{R}^3))$,
(ii) the infinitesimal plastic slips $\gamma^{\alpha} \in \mathrm{H}^1(0,T;L^2(\Omega))$ for $\alpha = 1,\dots,n_{\mathrm{slip}}$,
(iii) the hardening variables $\eta^{\alpha} \in \mathrm{H}^1(0,T;L^2(\Omega))$ for $\alpha = 1,\dots,n_{\mathrm{slip}}$,
(iv) the infinitesimal micro-distortion $\chi_p \in \mathrm{H}^1(0,T;H(\mathrm{Curl};\Omega,\mathbb{R}^{3\times 3}))$, with Curl Curl $\chi_p \in \mathrm{H}^1(0,T;L^2(\Omega,\mathbb{R}^{3\times 3}))$

such that the content of Table 2 holds.

3.2.5. Weak formulation of the model

Assume that the problem in Section 3.2.4 has a solution $(u,\underline{\gamma},\chi_p,\underline{\eta})$. We will extensively make use of the identity (3.4). Let $v \in H^1(\Omega,\mathbb{R}^3)$ with $v_{|\Gamma_D} = 0$. Multiply the equilibrium equation with $v - \dot{u}$ and integrate in space by parts and use the symmetry of σ and the elasticity relation to get

$$\int_{\Omega} \langle \mathbb{C}_{\mathrm{iso}}\mathrm{sym}(\nabla u - \overline{m}\,\underline{\gamma}), \mathrm{sym}(\nabla v - \nabla \dot{u})\rangle \, dx = \int_{\Omega} f(v-\dot{u})\, dx. \tag{3.37}$$

Now, for any $X \in C^{\infty}(\overline{\Omega},\mathfrak{sl}(3))$ such that $X \times n = 0$ on Γ_{D} we integrate (3.12) over Ω, integrate by parts the term with Curl Curl using the boundary conditions

$$(X-\dot{\chi}_p)\times n = 0 \text{ on } \Gamma_{\mathrm{D}}, \quad \mathrm{Curl}\,\chi_p \times\ n = 0 \text{ on } \partial\Omega \setminus \Gamma_{\mathrm{D}}$$

and get

$$\int_{\Omega} \Big[\mu\, L_c^2 \langle \mathrm{Curl}\,\chi_p, \mathrm{Curl}\,X - \mathrm{Curl}\,\dot{\chi}_p\rangle + \mu\, H_{\chi}\langle \chi_p - \overline{m}\,\underline{\gamma}, X - \dot{\chi}_p\rangle\Big] dx = 0. \tag{3.38}$$

Moreover, for any $\underline{q} = (q^1,\dots,q^{n_{\mathrm{slip}}})$ with $q^{\alpha} \in C^{\infty}(\overline{\Omega})$ and any $\underline{\beta} = (\beta^1,\dots,\beta^{n_{\mathrm{slip}}})$ with $\beta^{\alpha} \in L^2(\Omega)$, summing (3.36) over $\alpha = 1,\dots,n_{\mathrm{slip}}$ and integrating over Ω, we get

Table 2
The microcurl model in single crystal gradient plasticity with isotropic hardening.

Additive split of distortion:	$\nabla u = e + p$, $e_e = \mathrm{sym}\, e$, $e_p = \mathrm{sym}\, p$
Plastic distortion in slip system:	$p = \sum_{\alpha=1}^{n_{\mathrm{slip}}} \gamma^{\alpha}\, m^{\alpha}$ with $m^{\alpha} = l^{\alpha} \otimes \nu^{\alpha}$, $\mathrm{tr}(p) = 0$
Equilibrium:	$\mathrm{Div}\,\sigma + f = 0$ with $\sigma = \mathbb{C}_{\mathrm{iso}} e_e = \mathbb{C}_{\mathrm{iso}}(\mathrm{sym}\,\nabla u - e_p)$
Microbalance:	$\mu\, L_c^2\ \mathrm{Curl}\ \mathrm{Curl}\ \chi_p = -\mu\, H_{\chi}\ (\chi_p - p)$,
Free energy:	$\frac{1}{2}\langle \mathbb{C}_{\mathrm{iso}} e_e, e_e\rangle + \frac{1}{2}\mu\, H_{\chi}\|p-\chi_p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\mathrm{Curl}\,\chi_p\|^2 + \frac{1}{2}\mu\, k_2 \sum_{\alpha}|\eta^{\alpha}|^2$
Yield condition in α-th slip system:	$\lvert\tau^{\alpha}_{\mathrm{E}}\rvert + g^{\alpha} - \sigma_0 \leq 0$
where	$\tau^{\alpha}_{\mathrm{E}} := \langle \Sigma_E, m^{\alpha}\rangle$ with
	$\Sigma_E := \sigma + \mu\, H_{\chi}\ (\chi_p - p) = \sigma - \mu\, L_c^2\ \mathrm{Curl}\ \mathrm{Curl}\ \chi_p$
	$g^{\alpha} = -\mu\, k_2\ \eta^{\alpha}$
Dissipation inequality in α-th slip system:	$\tau^{\alpha}_{\mathrm{E}}\,\dot{\gamma}^{\alpha} + g^{\alpha}\,\dot{\eta}^{\alpha} \geq 0$
Dissipation function in α-th slip system:	$\mathscr{D}^{\alpha}_{\mathrm{iso}}(q^{\alpha},\beta^{\alpha}) := \begin{cases} \sigma_0\lvert q^{\alpha}\rvert & \text{if } \lvert q^{\alpha}\rvert \leq \beta^{\alpha}, \\ \infty & \text{otherwise} \end{cases}$
Flow rules in primal form:	$(\tau^{\alpha}_{\mathrm{E}}, g^{\alpha}) \in \partial \mathscr{D}^{\alpha}_{\mathrm{iso}}(\dot{\gamma}^{\alpha},\dot{\eta}^{\alpha})$
Flow rules in dual form:	$\dot{\gamma}^{\alpha} = \lambda^{\alpha}\frac{\tau^{\alpha}_{\mathrm{E}}}{\lvert\tau^{\alpha}_{\mathrm{E}}\rvert}, \quad \dot{\eta}^{\alpha} = \lambda^{\alpha} = \lvert\dot{\gamma}^{\alpha}\rvert$
KKT conditions:	$\lambda^{\alpha} \geq 0, \quad \phi(\tau^{\alpha}_E, g^{\alpha}) \leq 0, \quad \lambda^{\alpha}\,\phi(\tau^{\alpha}_E, g^{\alpha}) = 0$
Boundary conditions for χ_p:	$\chi_p \times n = 0$ on Γ_{D}, $(\mathrm{Curl}\,\chi_p)\times n = 0$ on $\partial\Omega\setminus\Gamma_{\mathrm{D}}$
Function space for χ_p:	$\chi_p(t,\cdot) \in \mathrm{H}(\mathrm{Curl};\ \Omega,\ \mathbb{R}^{3\times 3})$

$$\int_\Omega \mathscr{D}_{\rm iso}(\underline{q},\underline{\beta})\,dx - \int_\Omega \mathscr{D}_{\rm iso}(\dot{\underline{\gamma}},\dot{\underline{\eta}})dx - \int_\Omega \langle \mathbb{C}_{\rm iso}{\rm sym}(\nabla u - \overline{m}\underline{\gamma}), {\rm sym}(\overline{m}\underline{q} - \overline{m}\dot{\underline{\gamma}})\rangle dx + \int_\Omega \Big[-\mu H_\chi\langle \chi_p - \overline{m}\underline{\gamma}, \overline{m}\underline{q} - \overline{m}\dot{\underline{\gamma}}\rangle + \mu k_2\langle \underline{\eta}, \underline{\beta} - \dot{\underline{\eta}}\rangle\Big]dx \geq 0. \tag{3.39}$$

where

$$\mathscr{D}_{\rm iso}(\underline{q},\underline{\beta}) := \sum_\alpha \mathscr{D}^\alpha_{\rm iso}(q^\alpha,\beta^\alpha). \tag{3.40}$$

Now adding up (3.37)–(3.39) we get the following weak formulation of the problem set in Section 3.2.4 in the form of a variational inequality:

$$\int_\Omega \Big[\langle \mathbb{C}_{\rm iso}{\rm sym}(\nabla u - \overline{m}\,\underline{\gamma}), {\rm sym}(\nabla v - \overline{m}\,\underline{q}) - {\rm sym}(\nabla \dot{u} - \overline{m}\,\dot{\underline{\gamma}})\rangle + \mu\, L_c^2\langle {\rm Curl}\,\chi_p, {\rm Curl}\,X - {\rm Curl}\,\dot{\chi}_p\rangle + \mu\, H_\chi\langle \chi_p - \overline{m}\,\underline{\gamma}, (X - \overline{m}\,\underline{q}) - (\dot{\chi}_p - \overline{m}\,\dot{\underline{\gamma}})\rangle + \mu\, k_2\langle \underline{\eta}, \underline{\beta} - \dot{\underline{\eta}}\rangle\Big]dx + \int_\Omega \mathscr{D}_{\rm iso}(\underline{q},\underline{\beta})\,dx - \int_\Omega \mathscr{D}_{\rm iso}(\dot{\underline{\gamma}},\dot{\underline{\eta}})dx \geq \int_\Omega f(v-\dot{u})dx. \tag{3.41}$$

3.2.6. Existence result for the weak formulation

To prove the existence result for the weak formulation (3.41), we closely follow the abstract machinery developed by Han and Reddy in Han and Reddy (2013) for mathematical problems in geometrically linear classical plasticity and used for instance in Djoko et al. (2007a), Reddy et al. (2008), Neff et al. (2009a), Ebobisse and Neff (2010) and Ebobisse et al. (2016a, 2016b) for models of gradient plasticity. To this aim, Equation (3.41) is written as the variational inequality of the second kind: find $w = (u, \underline{\gamma}, \chi_p, \underline{\eta}) \in {\rm H}^1(0,T;{\rm Z})$ such that $w(0) = 0$, $\dot{w}(t) \in {\rm W}$ for a.e. $t \in [0,T]$ and

$$\boldsymbol{a}(w, z-\dot{w}) + j(z) - j(\dot{w}) \geq \langle \ell, z-\dot{w}\rangle \text{ for every } z \in {\rm W} \text{ and for a.e. } t \in [0,T], \tag{3.42}$$

where Z is a suitable Hilbert space and W is some closed, convex subset of Z to be constructed later,

$$\boldsymbol{a}(w,z) = \int_\Omega \Big[\langle \mathbb{C}_{\rm iso}{\rm sym}(\nabla u - \overline{m}\,\underline{\gamma}), {\rm sym}(\nabla v - \overline{m}\,\underline{q})\rangle + \mu\, L_c^2\langle {\rm Curl}\,\chi_p, {\rm Curl}\,X\rangle + \mu\, H_\chi\langle \chi_p - \overline{m}\,\underline{\gamma}, X - \overline{m}\,\underline{q}\rangle + \mu\, k_2\langle \underline{\eta}, \underline{\beta}\rangle\Big]dx, \tag{3.43}$$

$$j(z) = \int_\Omega \mathscr{D}_{\rm iso}(\underline{q},\underline{\beta})dx, \tag{3.44}$$

$$\langle \ell, z\rangle = \int_\Omega f\, v\, dx, \tag{3.45}$$

for $w = (u, \underline{\gamma}, \chi_p, \underline{\eta})$ and $z = (v, \underline{q}, X, \underline{\beta})$ in Z.

The Hilbert space Z and the closed convex subset W are constructed in such a way that the functionals $\boldsymbol{a}$, j and ℓ satisfy the assumptions in the abstract result in Han and Reddy (2013), Theorem 6.19. The key issue here is the coercivity of the bilinear form $\boldsymbol{a}$ on the set W, that is, $a(z,z) \geq C\|z\|_Z^2$ for every $z \in {\rm W}$ and for some $C > 0$.

We let

$${\rm V} := {\rm H}^1_0(\Omega, \Gamma_{\rm D}, \mathbb{R}^3) = \{v \in {\rm H}^1(\Omega, \mathbb{R}^3) \,|\, v_{|\Gamma_{\rm D}} = 0\}, \tag{3.46}$$

$${\rm P} := {\rm L}^2(\Omega, \mathbb{R}^{n_{\rm slip}}), \tag{3.47}$$

$${\rm Q} := {\rm H}_0({\rm Curl};\ \Omega,\ \Gamma_{\rm D}, \mathfrak{sl}(3)), \tag{3.48}$$

$$\Lambda := L^2(\Omega, \mathbb{R}^{n_{\rm slip}}), \tag{3.49}$$

$$\mathrm{Z} := \mathrm{V} \times \mathrm{P} \times \mathrm{Q} \times \Lambda, \tag{3.50}$$

$$\mathrm{W} := \left\{ z = (v, \underline{q}, X, \underline{\beta}) \in \mathrm{Z} \,|\, |q^\alpha| \leq \beta^\alpha, \quad \alpha = 1, \ldots, n_{\text{slip}} \right\}, \tag{3.51}$$

and define the norms

$$\begin{aligned} &\|v\|_V := \|\nabla v\|_{L^2}, \quad \|\underline{q}\|_P^2 = \sum_\alpha \|q^\alpha\|_{L^2}^2, \quad \|\underline{\beta}\|_\Lambda^2 = \sum_\alpha \|\beta^\alpha\|_{L^2}^2, \quad \|X\|_Q := \|X\|_{\mathrm{H(Curl;\Omega)}}, \\ &\|z\|_z^2 := \|v\|_V^2 + \|\underline{q}\|_P^2 + \|X\|_Q^2 + \|\underline{\beta}\|_\Lambda^2 \quad \text{for } z = (v, \underline{q}, X, \underline{\beta}) \in \mathrm{Z}. \end{aligned} \tag{3.52}$$

Let us show that the bilinear form $\boldsymbol{a}$ is coercive on W. Let therefore $z = (v, \underline{q}, X, \underline{\beta}) \in \mathrm{W}$.
First of all notice that

$$\|\overline{m}\, \underline{q}\|_{L^2} \leq \|\underline{q}\|_P \;\leq\; \|\underline{\beta}\|_\Lambda. \tag{3.53}$$

So,

$$\begin{aligned} \boldsymbol{a}(z,z) \quad &\geq m_0 \|\mathrm{sym}(\nabla v - \overline{m}\, \underline{q})\|_{L^2}^2 (\text{from}(2.3)) + \mu\, H_\chi \|X - \overline{m}\, \underline{q}\|_{L^2}^2 + \mu\, L_c^2 \|\mathrm{Curl}\, X\|_{L^2}^2 + \mu\, k_2 \|\underline{\beta}\|_\Lambda^2 \\ &= m_0 \left[\|\mathrm{sym}\nabla v\|_{L^2}^2 + \|\mathrm{sym}(\overline{m}\, \underline{q})\|_2^2 - 2\langle \mathrm{sym}\nabla v, \mathrm{sym}(\overline{m}\, \underline{q}) \rangle_{L^2} \right] + \mu\, H_\chi \left[\|X\|_{L^2}^2 + \|\overline{m}\, \underline{q}\|_{L^2}^2 - 2\langle X, \overline{m}\, \underline{q} \rangle_{L^2} \right] \\ &\quad + \mu L_c^2 \|\mathrm{Curl}\, X\|_{L^2}^2 + \mu\, k_2 \|\underline{\beta}\|_\Lambda^2 \\ &\geq m_0 \left[\|\mathrm{sym}\nabla v\|_{L^2}^2 + \|\mathrm{sym}(\overline{m}\, \underline{q})\|_{L^2}^2 - \theta \|\mathrm{sym}(\nabla v)\|_{L^2}^2 - \frac{1}{\theta} \|\mathrm{sym}(\overline{m}\, \underline{q})\|_{L^2}^2 \right] + \mu\, H_\chi \left[\|X\|_{L^2}^2 + \|\overline{m}\, \underline{q}\|_{L^2}^2 - \theta \|X\|_{L^2}^2 \right. \\ &\quad \left. - \frac{1}{\theta} \|\overline{m}\, \underline{q}\|_{L^2}^2 \right] (\text{Young's inequality}) + \mu\, L_c^2 \|\mathrm{Curl}\, X\|_{L^2}^2 + \frac{1}{2} \mu\, k_2 \|\underline{\beta}\|_\Lambda^2 + \frac{1}{2} \mu\, k_2\, \|\underline{q}\|_P^2 \quad (\text{using second} \\ &\quad \leq \text{in } (3.53)) \\ &= m_0 (1-\theta) \|\mathrm{sym}\nabla v\|_{L^2}^2 + m_0 \left(1 - \frac{1}{\theta} \right) \|\mathrm{sym}(\overline{m}\, \underline{q})\|_{L^2}^2 + \mu\, H_\chi \left(1 - \frac{1}{\theta} \right) \|\underline{q}\|_P^2 + \frac{1}{2} \mu\, k_2 \|\underline{q}\|_P^2 + \mu\, H_\chi (1-\theta) \|X\|_{L^2}^2 \\ &\quad + \mu\, L_c^2 \|\mathrm{Curl}\, X\|_2^2 + \frac{1}{2} \mu\, k_2 \|\underline{\beta}\|_\Lambda^2 \\ &\geq m_0 (1-\theta) \|\mathrm{sym}\nabla v\|_{L^2}^2 + \left[(m_0 + \mu\, H_\chi) \left(1 - \frac{1}{\theta} \right) + \frac{1}{2} \mu\, k_2 \right] \|\underline{q}\|_P^2 + \mu\, H_\chi (1-\theta) \|X\|_{L^2}^2 + \mu\, L_c^2 \|\mathrm{Curl}\, X\|_2^2 \\ &\quad + \frac{1}{2} \mu\, k_2 \|\underline{\beta}\|_\Lambda^2 \quad (\text{for } 0 < \theta < 1). \end{aligned} \tag{3.54}$$

So, since the hardening constant $k_2 > 0$, it is possible to choose θ such that

$$\frac{m_0 + \mu\, H_\chi}{m_0 + \mu\, H_\chi + \frac{1}{2} \mu\, k_2} < \theta < 1,$$

we always are able to find some constant $C(\theta, m_0, \mu, H_\chi, k_2, L_c, \Omega) > 0$ such that

$$a(z,z) \geq C \left[\|v\|_V^2 + \|\underline{q}\|_P^2 + \|X\|_{\mathrm{H(Curl;\Omega)}}^2 + \|\underline{\beta}\|_\Lambda^2 \right] = C \|z\|_Z^2 \quad \forall z = (v, \underline{q}, X, \underline{\beta}) \in \mathrm{W}. \tag{3.55}$$

This shows existence for the microcurl model in single gradient plasticity with isotropic hardening.

3.2.7. Uniqueness of the weak/strong solution

As shown in Ebobisse et al. (2016a) for a canonical rate-independent model of geometrically linear isotropic gradient plasticity with isotropic hardening and plastic spin, the uniqueness of the solution for our model can be obtained similarly. To this aim, notice that if $(u, \underline{\gamma}, \underline{\chi}_p, \underline{\eta})$ is a weak solution of the model, then $(u, \underline{\gamma}, \underline{\chi}_p, \underline{\eta})$ is also a strong solution. In fact, choosing appropriately test functions in the variational inequality (3.41), we obtain both equilibrium and microbalance equations on the one hand. The latter which is

$$\mu\, L_c^2\, \mathrm{Curl\,Curl}\, \chi_p = -\mu\, H_\chi(\chi_p - p)$$

is satisfied first in the distributional sense and hence is satisfied also in the L^2-sense since the right hand side is in $L^2(\Omega, \mathbb{R}^{3\times 3})$. Therefore, it follows that Curl Curl χ_p is also in $L^2(\Omega, \mathbb{R}^{3\times 3})$.

Now going back to (3.41), we also derive the boundary condition $(\mathrm{Curl}\,\chi_p)\times n|_{\partial\Omega\setminus\Gamma_D} = 0$ which is now justified because we derived that Curl $\chi_p \in \mathrm{H}(\mathrm{Curl};\ \Omega,\ \mathfrak{sl}(3))$.

On the other hand, we also obtain from (3.41) the following set of inequalities

$$\langle \dot{\Gamma}_p^\alpha, \Sigma^\alpha - \Sigma_p^\alpha\rangle \le 0 \quad \forall\, \Sigma^\alpha \in \mathscr{K}^\alpha, \quad \alpha = 1, \dots, n_{\mathrm{silp}} \tag{3.56}$$

and hence, $(u, \underline{\gamma}, \chi_p, \underline{\eta})$ is a strong solution.

Now let us consider two solutions $w_i := (u_i, \underline{\gamma_i}, \chi_{p\,i}, \underline{\eta_i})$, $i = 1, 2$ of (3.41) satisfying the same initial conditions, let $\Gamma_{p_i}^\alpha = (\gamma_i^\alpha, \eta_i^\alpha)$ and let $\Sigma_{p_i}^\alpha := (\tau_{E_i}^\alpha, g_i^\alpha)$ be the corresponding stresses. That is,

$$\tau_{E_i}^\alpha = \langle \Sigma_{E_i}, m^\alpha\rangle = \langle \sigma_i + \mu\, H_\chi(\chi_{p_i} - p_i), m^\alpha\rangle = \langle \sigma_i - \mu\, H_\chi \mathrm{Curl\,Curl}\, \chi_{p_i}, m^\alpha\rangle, \tag{3.57}$$

$$g_i^\alpha = -\mu\, k_2\, \eta_i^\alpha \tag{3.58}$$

so that $\Gamma_{p_i}^\alpha$ and $\Sigma_{p_i}^\alpha$ satisfy

$$\langle \dot{\Gamma}_{p_1}^\alpha, \Sigma^\alpha - \Sigma_{p_1}^\alpha\rangle \le 0 \quad \text{and} \quad \langle \dot{\Gamma}_{p_2}^\alpha, \Sigma^\alpha - \Sigma_{p_2}^\alpha\rangle \le 0 \quad \forall\, \Sigma^\alpha \in \mathscr{K}^\alpha. \tag{3.59}$$

Now choose $\Sigma^\alpha = \Sigma_{p_2}^\alpha$ in $(3.59)_1$ and $\Sigma^\alpha = \Sigma_{p_1}^\alpha$ in $(3.59)_2$ and add up to get

$$\langle \Sigma_{p_2}^\alpha - \Sigma_{p_1}^\alpha, \dot{\Gamma}_{p_1}^\alpha - \dot{\Gamma}_{p_2}^\alpha\rangle \le 0. \tag{3.60}$$

That is,

$$\langle \sigma_2 - \sigma_1, m^\alpha\, \dot{\gamma}_1^\alpha - m^\alpha\, \dot{\gamma}_2^\alpha\rangle + \mu\, H_\chi\langle (\chi_{p\,2} - \chi_{p\,1}) - (p_2 - p_1), m^\alpha\, \dot{\gamma}_1^\alpha - m^\alpha\, \dot{\gamma}_2^\alpha\rangle + (g_2^\alpha - g_1^\alpha)(\dot{\eta}_1^\alpha - \dot{\eta}_2^\alpha) \le 0 \tag{3.61}$$

and adding up over α, we get

$$\langle \sigma_2 - \sigma_1, \dot{p}_1 - \dot{p}_2\rangle + \mu\, H_\chi\langle (\chi_{p\,2} - \chi_{p\,1}) - (p_2 - p_1), \dot{p}_1 - \dot{p}_2\rangle + \langle \underline{g_2} - \underline{g_1}, \underline{\dot{\eta}_1} - \underline{\dot{\eta}_2}\rangle \le 0 \tag{3.62}$$

Now, substitute $\mathrm{sym}\, p_i = \mathrm{sym}\nabla u_i - \mathbb{C}_{\mathrm{iso}}^{-1}\sigma_i$ obtained from the elasticity relation, into the expression $\langle \sigma_2 - \sigma_1, \dot{p}_1 - \dot{p}_2\rangle$ and $\dot{p}_i = \dot{\chi}_{p_i} + \frac{L_c^2}{H_\chi}\,\mathrm{Curl\,Curl}\,\dot{\chi}_{p\,i}$ obtained from the microbalance equation into the expression $\langle \chi_{p_2} - \chi_{p_1}, \dot{p}_1 - \dot{p}_2\rangle$ and get from (3.62) that

$$\begin{aligned}\langle \sigma_2 - \sigma_1, \mathbb{C}_{\mathrm{iso}}^{-1}(\dot{\sigma}_2 - \dot{\sigma}_1)\rangle + \mu\, H_\chi\langle p_1 - p_2, \dot{p}_1 - \dot{p}_2\rangle + \mu\, H_\chi\langle \chi_{p_2} - \chi_{p_1}, \dot{\chi}_{p_1} - \dot{\chi}_{p_2}\rangle + \mu\, L_c^2\langle \chi_{p_2} - \chi_{p_1}, \mathrm{Curl\,Curl}\,\chi_{p_1}\\ - \mathrm{Curl\,Curl}\,\chi_{p_2}\rangle + \langle \underline{g_2} - \underline{g_1}, \underline{\dot{\eta}_1} - \underline{\dot{\eta}_2}\rangle \le \langle \sigma_1 - \sigma_2, \mathrm{sym}(\nabla u_1) - \mathrm{sym}(\nabla u_2)\rangle\end{aligned} \tag{3.63}$$

Now for every $t \in [0, T]$, we integrate (3.63) over $\Omega \times (0, t)$ using the boundary conditions on $\chi_{p\,i}$ and using the fact that

$$\int_\Omega \langle \sigma_1 - \sigma_2, \mathrm{sym}(\nabla u_1) - \mathrm{sym}(\nabla u_2)\rangle dx = 0,$$

we get

$$\int_0^t \frac{d}{ds}\Big[\|\mathbb{C}_{\rm iso}^{-1/2}(\sigma_2(s)-\sigma_1(s))\|_{L^2}^2+\mu\, H_\chi\|p_1(s)-p_2(s)\|_{L^2}^2-\mu\, H_\chi\|\chi_{p_2}(s)-\chi_{p_1}(s)\|_{L^2}^2-\mu\, L_c^2\|\mathrm{Curl}\,\chi_{p_2}(s)-\mathrm{Curl}\,\chi_{p_1}(s)\|_{L^2}^2$$
$$+\mu\, k_2\|\underline{\eta_1}(s)-\underline{\eta_2}(s)\|_{L^2}^2\Big]\,ds\le 0.$$

Therefore, we obtain

$$\|\mathbb{C}_{\rm iso}^{-1/2}(\sigma_2-\sigma_1)\|_{L^2}^2+\mu\, H_\chi\|p_1-p_2\|_{L^2}^2+\mu\, k_2\|\underline{\eta_1}-\underline{\eta_2}\|_{L^2}^2\le \mu\, H_\chi\|\chi_{p_2}-\chi_{p_1}\|_{L^2}^2+\mu\, L_c^2\|\mathrm{Curl}\,\chi_{p_2}-\mathrm{Curl}\,\chi_{p_1}\|_{L^2}^2. \tag{3.64}$$

On the other hand, we write the micro-balance equation for p_i and χ_{p_i} with $i=1,2$, as

$$\mu\, H_\chi\, p_1=\mu\, L_c^2\,\mathrm{Curl}\,\mathrm{Curl}\,\chi_{p_1}+\mu\, H_\chi\chi_{p_1}, \tag{3.65}$$

$$\mu\, H_\chi\, p_2=\mu\, L_c^2\,\mathrm{Curl}\,\mathrm{Curl}\,\chi_{p_2}+\mu\, H_\chi\chi_{p_2}, \tag{3.66}$$

then we subtract, take the scalar product with $\chi_{p_1}-\chi_{p_2}$, integrate using the boundary condition

$$(\chi_{p_1}-\chi_{p_2})\times n|_{\Gamma_{\rm D}}=0\quad\text{and}\quad(\mathrm{Curl}\,\chi_{p_1}-\mathrm{Curl}\,\chi_{p_2})\times n|_{\partial\Omega\setminus\Gamma_{\rm D}}=0$$

and get

$$\mu\, H_\chi\int_\Omega\langle p_1-p_2,\chi_{p_1}-\chi_{p_2}\rangle dx=\mu\, L_c^2\|\mathrm{Curl}\,\chi_{p_1}-\mathrm{Curl}\,\chi_{p_2}\|_{L^2}^2+\mu\, H_\chi\|\chi_{p_1}-\chi_{p_2}\|_{L^2}^2. \tag{3.67}$$

Therefore, we obtain from (3.64) and (3.67) that

$$\mu\, H_\chi\|p_1-p_2\|_{L^2}^2\le\mu\, L_c^2\|\mathrm{Curl}\,\chi_{p_1}-\mathrm{Curl}\,\chi_{p_2}\|_{L^2}^2+\mu\, H_\chi\|\chi_{p_1}-\chi_{p_2}\|_{L^2}^2 \tag{3.68}$$

$$\le\mu\, H_\chi\|p_1-p_2\|_{L^2}\|\chi_{p_1}-\chi_{p_2}\|_{L^2} \tag{3.69}$$

which implies that

$$\|p_1-p_2\|_{L^2}=\|\chi_{p_1}-\chi_{p_2}\|_{L^2}\quad\text{and hence,}\quad\|\mathrm{Curl}\,\chi_{p_1}-\mathrm{Curl}\,\chi_{p_2}\|_{L^2}=0. \tag{3.70}$$

Now, going back to (3.64), we get

$$\|\mathbb{C}_{\rm iso}^{-1/2}(\sigma_2-\sigma_1)\|_{L^2}^2+\mu\, k_2\|\underline{\eta_1}-\underline{\eta_2}\|_{L^2}^2\le 0. \tag{3.71}$$

Hence, we obtain so far,

$$\sigma_1-\sigma_2,\quad\underline{\eta_1}=\underline{\eta_2}\quad\text{and}\quad\mathrm{Curl}\,\chi_{p_1}=\mathrm{Curl}\,\chi_{p_2}\quad\Rightarrow\quad\tau_{E_1}^\alpha=\tau_{E_2}^\alpha.$$

Now, let us prove that $\gamma_1^\alpha=\gamma_2^\alpha$ for every α. In fact, from the definition of the normal cone it follows that $\dot\Gamma_{p_i}^\alpha=0$ that is, $\dot\gamma_i^\alpha=\dot\eta_i^\alpha=0$ inside the elastic domain $\mathrm{Int}(\mathscr{K}^\alpha)$ (for the α-slip system), which from the initial conditions imply that $\gamma_i^\alpha=0$ inside $\mathrm{Int}(\mathscr{K}^\alpha)$. Now, looking at the flow rule in dual form (for the α-slip system) in Table 2, we obtain from $\tau_{E_1}^\alpha=\tau_{E_2}^\alpha$ that $\dot\gamma_1^\alpha=\dot\gamma_2^\alpha$ which implies that $\gamma_1^\alpha=\gamma_2^\alpha$ from the initial conditions. Therefore, we obtain $p_1=p_2$ which implies from $(3.70)_1$ that $\chi_{p_1}=\chi_{p_2}$.

Now, it remains to show that $u_1=u_2$. This is obtained exactly as in Ebobisse et al. (2016a). We repeat the proof here just for the reader's convenience. To this end, we use $\mathrm{sym}(\nabla u_i)=\mathbb{C}^{-1}\sigma_i+\mathrm{sym}p_i$ obtained from the elasticity relation and get

$$\mathrm{sym}(\nabla(u_1-u_2))=\mathbb{C}^{-1}(\sigma_1-\sigma_2)+\mathrm{sym}(p_1-p_2)=0,$$

and hence, from the first Korn's inequality (see e.g. Neff, 2002), we get $\nabla(u_1-u_2)=0$ which implies that $u_1=u_2$. Therefore, we finally obtain

$$u_1 = u_2, \quad \sigma_1 = \sigma_2, \quad \big(\underline{\gamma_1} = \underline{\gamma_2} \quad \Rightarrow \quad p_1 = p_2\big), \quad \chi_{p_1} = \chi_{p_2}, \quad \underline{\eta_1} = \underline{\eta_2},$$

and thus the uniqueness of a weak/strong solution.

Remark 3.1. It should be stressed that, in the proof, $k_2 > 0$ is necessary for uniqueness of the displacement field (and of the slip variables). If $k_2 = 0$, we have perfect plasticity and multiple solutions involving displacement discontinuities along *slip lines*, as in conventional Hill's plasticity, are possible. The curl operator does not regularize such discontinuities since curl p may vanish in the presence of gradient of slip γ^α perpendicularly to the slip planes. It is shown in Forest (1998) that gradient models lead to finite width *kink bands* but still allow for *slip band* discontinuities, parallel to slip planes, in single crystals.

3.3. The model with linear kinematical hardening

Here we consider the model where the isotropic hardening has been replaced with linear kinematical hardening.

3.3.1. The description of the model

Here the free-energy density Ψ is also given in the additively separated form as

$$\Psi(\nabla u, p, \chi_p, \operatorname{Curl}\chi_p) := \underbrace{\Psi^{\rm lin}_e(\varepsilon_e)}_{\text{elastic energy}} + \underbrace{\Psi^{\rm lin}_{\rm micro}(p,\chi_p)}_{\text{micro energy}} + \underbrace{\Psi^{\rm lin}_{\rm curl}(\operatorname{Curl}\chi_p)}_{\text{defect-like energy (GND)}} + \underbrace{\Psi^{\rm lin}_{\rm kin}(\varepsilon_p)}_{\text{hardening energy (SSD)}}, \tag{3.72}$$

where

$$\begin{aligned} \Psi^{\rm lin}_e(\varepsilon_e) &:= \frac{1}{2}\langle \varepsilon_e, \mathbb{C}_{\rm iso}\varepsilon_e\rangle = \frac{1}{2}\langle \operatorname{sym}(\nabla u - p), \mathbb{C}_{\rm iso}\operatorname{sym}(\nabla u - p)\rangle, \\ \Psi^{\rm lin}_{\rm micro}(p,\chi_p) &:= \frac{1}{2}\mu\, H_\chi \|p - \chi_p\|^2, \quad \Psi^{\rm lin}_{\rm curl}(\operatorname{Curl}\chi_p) := \frac{1}{2}\mu\, L_c^2 \|\operatorname{Curl}\chi_p\|^2, \\ \Psi^{\rm lin}_{\rm kin}(\varepsilon_p) &:= \frac{1}{2}\mu\, k_1 \|\varepsilon_p\|^2 = \frac{1}{2}\mu\, k_1 \|\operatorname{sym} p\|^2. \end{aligned} \tag{3.73}$$

In this case, the equilibrium equation and the microcurl balance are obtained as in (3.10) and in (3.12) respectively.

Now, the free-energy imbalance

$$\dot\Psi \le \langle \sigma, \nabla u\rangle = \langle \sigma, \dot\varepsilon_e\rangle + \langle \sigma, \dot p\rangle$$

and the expansion of $\dot\Psi$ lead to the usual infinitesimal elastic stress-strain relation

$$\sigma = 2\mu\, \operatorname{sym}(\nabla u - p) + \lambda\, \operatorname{tr}(\nabla u - p)\mathbb{1} = 2\mu\big(\operatorname{sym}(\nabla u) - \varepsilon_p\big) + \lambda\, \operatorname{tr}(\nabla u)\mathbb{1}$$

and the local reduced dissipation inequality

$$\langle \Sigma_E, \dot p\rangle \ge 0, \tag{3.74}$$

where the non-symmetric Eshelby-type stress tensor in this case takes the form

$$\Sigma_E := \sigma + \Sigma^{\rm lin}_{\rm micro} + \Sigma^{\rm lin}_{\rm kin} \tag{3.75}$$

with

$$\Sigma^{\rm lin}_{\rm micro} := \mu\, H_\chi(\chi_p - p) = -\mu\, L_c^2 \operatorname{Curl}\operatorname{Curl}\chi_p, \tag{3.76}$$

$$\Sigma^{\rm lin}_{\rm kin} := -\mu\, k_1\, \varepsilon_p = -\mu\, k_1\, \operatorname{sym} p. \tag{3.77}$$

Two sources of kinematic hardening therefore arise in the model: the size–dependent contribution, $\Sigma^{\rm lin}_{\rm micro}$, induced by strain gradient plasticity, and conventional size–independent linear kinematic hardening $\Sigma^{\rm lin}_{\rm kin}$.

Following the steps in the derivation of the strong formulation of the microcurl model with isotropic hardening in Section 3.2.4, we get the strong formulation in Table 3 for the model with linear kinematical hardening.

3.3.2. The weak formulation of the model with linear kinematical hardening

The equilibrium and microbalance equations in weak form are

Table 3
The microcurl model in single crystal gradient plasticity with linear kinematical hardening.

Additive split of distortion:	$\nabla u = e + p$, $\varepsilon_e = \operatorname{sym} e$, $\varepsilon_p = \operatorname{sym} p$
Equilibrium:	$\operatorname{Div}\sigma + f = 0$ with $\sigma = \mathbb{C}_{\rm iso}\varepsilon_e = \mathbb{C}_{\rm iso}(\operatorname{sym}\nabla u - \varepsilon_p)$
Microbalance:	$\mu\, L_c^2 \operatorname{Curl}\operatorname{Curl}\chi_p = -\mu\, H_\chi(\chi_p - p)$,
Free energy:	$\frac{1}{2}\langle \mathbb{C}_{\rm iso}\varepsilon_e, \varepsilon_e\rangle + \frac{1}{2}\mu\, H_\chi \|p - \chi_p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\operatorname{Curl}\chi_p\|^2 + \frac{1}{2}\mu\, k_1 \|\operatorname{sym} p\|^2$
Yield condition:	$\phi(\Sigma_E) := \|\operatorname{dev}\Sigma_E\| - \sigma_0 \le 0$
where	$\Sigma_E := \sigma + \mu\, H_\chi(\chi_p - p) - \mu\, k_1 \operatorname{sym} p$
Dissipation inequality:	$\langle \Sigma_E, \dot p\rangle \ge 0$
Dissipation function:	$\mathscr{D}_{\rm iso}(q) := \sigma_0 \|q\|$
Flow rule in primal form:	$\Sigma_E \in \partial \mathscr{D}_{\rm iso}(\dot p)$
Flow rule in dual form:	$\dot p = \lambda \frac{\operatorname{dev}\Sigma_E}{\|\operatorname{dev}\Sigma_E\|}, \qquad \lambda = \|\dot p\|$
KKT conditions:	$\lambda \ge 0, \quad \phi(\Sigma_E, g) \le 0, \quad \lambda\,\phi(\Sigma_E, g) = 0$
Boundary conditions for χ_p:	$\chi_p \times n = 0$ on $\Gamma_{\rm D}$, $(\operatorname{Curl}\chi_p)\times n = 0$ on $\partial\Omega \setminus \Gamma_{\rm D}$
Function space for χ_p:	$\chi_p(t,\cdot) \in \mathrm{H}(\operatorname{Curl}; \Omega, \mathbb{R}^{3\times 3})$

$$\int_\Omega \langle \mathbb{C}_{\rm iso}\big(\operatorname{sym}\nabla u - \varepsilon_p\big), \operatorname{sym}(\nabla v - \nabla \dot u)\rangle dx = \int_\Omega f(v - \dot u) dx, \tag{3.78}$$

$$\int_\Omega \Big[\mu\, L_c^2 \langle \operatorname{Curl}\chi_p, \operatorname{Curl} X - \operatorname{Curl}\dot\chi_p\rangle + \mu\, H_\chi\langle \chi_p - p, X - \dot\chi_p\rangle\Big]\, dx = 0, \tag{3.79}$$

for every $v \in \mathrm{V}$ and $X \in \mathrm{Q}$ with V and Q defined in (3.46) and in (3.48), respectively.

Now, the primal formulation of the flow rule ($\Sigma_E \in \partial\mathscr{D}_{\rm kin}(\dot p)$) in weak form reads for every $q \in L^2(\Omega, \mathfrak{sl}(3))$ as

$$\begin{aligned}\int_\Omega \mathscr{D}_{\rm kin}(q)dx - \int_\Omega \mathscr{D}_{\rm kin}(\dot p)dx \;&\ge \int_\Omega \langle \Sigma_E, q - \dot p\rangle dx \\ &= \int_\Omega \langle \mathbb{C}_{\rm iso}\operatorname{sym}(\nabla u - p), \operatorname{sym}(q - \dot p)\rangle dx + \int_\Omega \Big[\langle \mu\, H_\chi\big(\chi_p - p\big) - \mu\, k_1 \operatorname{sym} p, q - \dot p\rangle\Big] dx.\end{aligned} \tag{3.80}$$

Now adding up (3.78), (3.79) and (3.80) we get the following weak formulation of the microcurl model of single crystal strain gradient plasticity with linear kinematical hardening in the form of a variational inequality:

$$\begin{aligned}\int_\Omega \Big[&\langle \mathbb{C}_{\rm iso}\operatorname{sym}(\nabla u - p), \operatorname{sym}(\nabla v - q) - \operatorname{sym}(\nabla \dot u - \dot p)\rangle + \mu\, L_c^2\langle \operatorname{Curl}\chi_p, \operatorname{Curl} X - \operatorname{Curl}\dot\chi_p\rangle + \mu\, H_\chi\langle \chi_p - p, (X - q)\\ &- (\dot\chi_p - \dot p)\rangle + \mu\, k_1\langle \operatorname{sym} p, \operatorname{sym}(q - \dot p)\rangle\Big] dx + \int_\Omega \mathscr{D}_{\rm kin}(q)dx - \int_\Omega \mathscr{D}_{\rm kin}(\dot p)dx \ge \int_\Omega f(v - \dot u)dx.\end{aligned} \tag{3.81}$$

That is, setting $\mathrm{Z} := \mathrm{V}\times\mathrm{P}\times\mathrm{Q}$ with V, P and Q defined in (3.46)–(3.48) and their norms in (3.52), we get the problem of the form: Find $w = (u, p, \chi_p) \in \mathrm{H}^1(0, T; Z)$ such that $w(0) = 0$ and

$$\boldsymbol{a}(w, z - \dot w) + j(z) - j(\dot w) \ge \langle \ell, z - \dot w\rangle \text{ for every } z \in \mathrm{Z} \text{ and for a.e. } t \in [0, T], \tag{3.82}$$

where

$$\boldsymbol{a}(w, z) := \int_\Omega \Big[\langle \mathbb{C}_{\rm iso}\operatorname{sym}(\nabla u - p), \operatorname{sym}(\nabla v - q)\rangle + \mu\, L_c^2\langle \operatorname{Curl}\chi_p, \operatorname{Curl} X\rangle + \mu\, H_\chi\langle \chi_p - p, X - q\rangle + \mu\, k_1\langle \operatorname{sym} p, \operatorname{sym} q\rangle\Big] dx, \tag{3.83}$$

$$j(z) := \int_\Omega \mathscr{D}_{\rm kin}(q)\, dx, \tag{3.84}$$

$$\langle \ell, z\rangle := \int_\Omega f\, v\, dx, \tag{3.85}$$

for $w = (u, p, \chi_p)$ and $z = (v, q, \mathrm{Q})$ in Z.

3.3.3. Existence and uniqueness for the model with linear kinematic hardening

In order to show the existence and uniqueness for the problem in (3.82)–(3.85) using Han and Reddy, 2013, Theorem 6.15, we only need to show here that the bilinear form $\boldsymbol{a}$ is Z-coercive. However, this is obtained following a different approach. We will make use of the following result.

Lemma 3.1. *The mapping* $\|\cdot\|_* : \mathrm{P}\times\mathrm{Q}\to[0,\infty)$ *defined by*

$$\|(q,X)\|_*^2 := \|q-X\|_{L^2}^2 + \|\mathrm{sym}\, q\|_{L^2}^2 + \|\mathrm{Curl}\, X\|_{L^2}^2 \tag{3.86}$$

is a norm on $\mathrm{P}\times\mathrm{Q}$ *equivalent to the norm defined by*

$$\|(q,X)\|_{P\times Q}^2 = \|q\|_{L^2}^2 + \|X\|_{\mathrm{H(Curl};\Omega)}^2. \tag{3.87}$$

Proof. To show that $\|\cdot\|_*$ is a norm on $\mathrm{P}\times\mathrm{Q}$, we only check the vanishing property of a norm since the other properties are trivially satisfied. The vanishing property is obtained through the Korn-type inequality for incompatible tensor fields established in Neff et al. (2011), 2012a, 2012b, 2014b, namely

$$\|X\|_{L^2}^2 \le C\big(\|\mathrm{sym}\, X\|_{L^2}^2 + \|\mathrm{Curl}\, X\|_{L^2}^2\big) \quad \forall X\in\mathrm{Q} := \mathrm{H}_0\big(\mathrm{Curl};\Omega,\Gamma_{\mathrm{D}},\mathbb{R}^{3\times3}\big). \tag{3.88}$$

In fact, let $(q,X)\in\mathrm{P}\times\mathrm{Q}$ be such that $\|(q,X)\|_* = 0$, that is, $q = X$, $\mathrm{sym}\, q = 0$ and $\mathrm{Curl}\, X = 0$.
Thus we get $\mathrm{sym}\, X = 0$ and $\mathrm{Curl}\, X = 0$. From (3.88), we then get $X = 0$ and hence also $q = 0$.
Now to show that both norms are equivalent, we will first show that $(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_*)$ is a Banach space. To this aim, let (q_n, X_n) be a Cauchy sequence in $(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_*)$. Hence, the sequences $(q_n - X_n)$, $(\mathrm{sym}\, q_n)$ and $(\mathrm{Curl}\, X_n)$ are all Cauchy in $L^2(\Omega,\mathbb{R}^{3\times3})$ and therefore, there exist $A,\ B,\ C\in L^2(\Omega,\mathbb{R}^{3\times3})$ such that

$$q_n - X_n\to A, \quad \mathrm{sym}\, q_n\to B, \quad \text{and} \quad \mathrm{Curl}\, X_n\to C. \tag{3.89}$$

Thus,

$$\mathrm{sym}\, X_n = \mathrm{sym}\, q_n - \mathrm{sym}(q_n - X_n)\to B - \mathrm{sym}\, A = \mathrm{sym}(B - A) \quad \text{and} \quad \mathrm{Curl}\, X_n\to C.$$

Hence, it follows from the inequality (3.88) that (X_n) is a Cauchy sequence in $(\mathrm{Q}, \|\cdot\|_{\mathrm{H(Curl};\Omega)})$.
Hence, there exists $X\in\mathrm{Q}$ such that

$$X_n\to X \quad \text{and} \quad \mathrm{Curl}\, X_n\to\mathrm{Curl}\, X = C \ \text{ in } \ L^2\big(\Omega,\mathbb{R}^{3\times3}\big).$$

Now $q_n = X_n + (q_n - X_n)\to X + A$ and $\mathrm{sym}\, q_n\to\mathrm{sym}(X + A) = B$. Therefore,

$$\begin{aligned}\|(q_n,X_n) - (X + A, X)\|_*^2 &= \|(q_n - (X + A), X_n - X)\|_*^2\\ &= \|(q_n - X_n) - A\|_{L^2}^2 + \|\mathrm{sym}\, q_n - \mathrm{sym}(X + A)\|_{L^2}^2 + \|\mathrm{Curl}\, X_n - \mathrm{Curl}\, X\|_{L^2}^2\to 0.\end{aligned}$$

So, the sequence (q_n, X_n) converges to $(X + A, X)$ in $(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_*)$.
Since the two normed spaces $(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_{P\times Q})$ and $(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_*)$ are Banach and the identity mapping

$$\mathrm{Id} : \big(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_{P\times Q}\big)\to(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_*)$$

is linear and continuous, then as a consequence of the open mapping theorem, we find that

$$\mathrm{Id} : (\mathrm{P}\times\mathrm{Q}, \|\cdot\|_*)\to\big(\mathrm{P}\times\mathrm{Q}, \|\cdot\|_{P\times Q}\big)$$

is also linear and continuous. Therefore, the two norms $\|\cdot\|_*$ and $\|\cdot\|_{P\times Q}$ are equivalent and this completes the proof of the lemma.

We are now in a position to prove that the bilinear form $\boldsymbol{a}$ in (3.84) is Z-coercive.

Lemma 3.2. *There exists a positive constant C such that $\boldsymbol{a}(z,z) \geq C\|z\|_Z^2$ for every $z \in Z$.*

Proof. Let $z = (v, q, X) \in Z = V \times P \times Q$

$$\begin{aligned}\boldsymbol{a}(z,z) &\geq m_0\|\mathrm{sym}(\nabla v - q)\|_{L^2}^2 (\text{from (2.3)}) + \mu\, H_\chi\|X - q\|_{L^2}^2 + \mu\, L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2 + \mu\, k_1\|\mathrm{sym}\, q\|_{L^2}^2\\ &= m_0\left[\|\mathrm{sym}\,\nabla v\|_{L^2}^2 + \|\mathrm{sym}\, q\|_{L^2}^2 - 2\langle \mathrm{sym}\,\nabla v, \mathrm{sym}\, q\rangle\right] + \mu\, H_\chi\|X - q\|_{L^2}^2 + \mu L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2 + \mu\, k_1\|\mathrm{sym}\, q\|_{L^2}^2\\ &\geq m_0(1-\theta)\|\mathrm{sym}\nabla v\|_{L^2}^2 + \left[m_0\left(1 - \frac{1}{\theta}\right) + \mu\, k_1\right]\|\mathrm{sym}\, q\|_2^2 + \mu\, H_\chi\|X - q\|_{L^2}^2 + \mu L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2.\end{aligned}$$

Now, since the hardening constant $k_1 > 0$, we choose θ such that

$$\frac{m_0}{m_0 + \mu\, k_1} < \theta < 1,$$

and using Korn's first inequality (see e.g. Neff, 2002) and Lemma 3.1, we then get two constants $C = C(\theta, m_0, \mu, H_\chi, k_1, L_c, \Omega) > 0$ and $C' = C'(\theta, m_0, \mu, H_\chi, k_1, L_c, \Omega) > 0$ such that

$$\boldsymbol{a}(z,z) \geq C'\left[\|\nabla v\|_{L^2}^2 + \|(q,X)\|_*^2\right] \geq C\left[\|\nabla v\|_{L^2}^2 + \|q\|_{L^2}^2 + \|X\|_{H(\mathrm{Curl};\Omega)}^2\right] = C\|z\|_Z^2.$$

4. The microcurl model in polycrystalline gradient plasticity

4.1. The case with isotropic hardening

The free-energy density Ψ is given in the additively separated form

$$\Psi(\nabla u, \varepsilon_p, \chi_p, \mathrm{Curl}\chi_p, \eta_p) := \underbrace{\Psi_e^{\mathrm{lin}}(\varepsilon_e)}_{\text{elastic energy}} + \underbrace{\Psi_{\mathrm{micro}}^{\mathrm{lin}}(\varepsilon_p, \chi_p)}_{\text{micro energy}} + \underbrace{\Psi_{\mathrm{curl}}^{\mathrm{lin}}(\mathrm{Curl}\,\chi_p)}_{\text{defect–like energy (GND)}} + \underbrace{\Psi_{\mathrm{iso}}^{\mathrm{lin}}(\eta_p)}_{\text{hardening energy (SSD)}}, \tag{4.1}$$

where

$$\begin{aligned}\Psi_e^{\mathrm{lin}}(\varepsilon_e) &:= \frac{1}{2}\langle \varepsilon_e, \mathbb{C}_{\mathrm{iso}}\varepsilon_e\rangle = \frac{1}{2}\langle \mathrm{sym}\nabla u - \varepsilon_p, \mathbb{C}_{\mathrm{iso}}(\mathrm{sym}\nabla u - \varepsilon_p)\rangle,\\ \Psi_{\mathrm{micro}}^{\mathrm{lin}}(\varepsilon_p, \chi_p) &:= \frac{1}{2}\mu\, H_\chi\|\varepsilon_p - \mathrm{sym}\,\chi_p\|^2, \quad \Psi_{\mathrm{curl}}^{\mathrm{lin}}(\mathrm{Curl}\,\chi_p) := \frac{1}{2}\mu\, L_c^2\|\mathrm{Curl}\,\chi_p\|^2,\\ \Psi_{\mathrm{iso}}^{\mathrm{lin}}(\eta_p) &:= \frac{1}{2}\mu\, k_2|\eta_p|^2.\end{aligned} \tag{4.2}$$

Here, η_p is the isotropic hardening variable.

It should be noted that there is no constraint on the skew–symmetric part of the microdeformation, skew χ_p, in (4.2), due to the fact that no plastic spin is considered in the original plasticity model for skew χ_p to be compared with. It will be shown that, in spite of that, no indeterminacy of skew χ_p arises in the formulation.[5] This represents the most straightforward microcurl extension of a phenomenological polycrystal plasticity model.

4.1.1. The balance equations

As in Section 3.2.1, we have the balance equations:

$$\mathrm{div}\,\sigma + f = 0 \quad (\text{macroscopic balance}), \tag{4.3}$$

$$\mu\, L_c^2\mathrm{Curl}\,\mathrm{Curl}\,\chi_p = \quad -\mu\, H_\chi(\mathrm{sym}\,\chi_p - \varepsilon_p) \in \mathrm{Sym}(3) \quad (\text{microbalance}), \tag{4.4}$$

where (4.4) is supplemented by the boundary conditions

[5] No simple characterization of skew χ_p for $H_\chi \to \infty$ is known at present.

$$\chi_p \times n|_{\Gamma_D} = 0 \quad \text{and} \quad (\text{Curl}\ \chi_p) \times n|_{\partial\Omega \setminus \Gamma_D} = 0. \tag{4.5}$$

4.1.2. The derivation of the dissipation inequality

The local free-energy imbalance states that

$$\dot{\Psi} - \langle \sigma, \dot{e}_e \rangle - \langle \sigma, \dot{e}_p \rangle \leq 0. \tag{4.6}$$

Now we expand the first term, substitute (4.1) and get

$$\langle \mathbb{C}_{\text{iso}}\, e_e - \sigma, \dot{e}_e \rangle - \langle \sigma, \dot{e}_p \rangle - \mu\, H_\chi \langle \text{sym}\, \chi_p - e_p, \dot{e}_p \rangle + \mu\, k_2\, \eta_p\, \dot{\eta}_p \leq 0. \tag{4.7}$$

Since the inequality (4.7) must be satisfied for whatever elastic-plastic deformation mechanism, inlcuding purely elastic ones (for which $\dot{\eta}_p = 0$, $\dot{e}_p = 0$), then it implies the infinitesimal stress-strain relation

$$\sigma = \mathbb{C}_{\text{iso}}\, e_e = 2\mu(\text{sym}\nabla u - e_p) + \lambda\, \text{tr}(\text{sym}\nabla u - e_p)\mathbb{1} \tag{4.8}$$

and the local reduced dissipation inequality

$$-\langle \sigma, \dot{e}_p \rangle - \mu\, H_\chi \langle \text{sym}\, \chi_p - e_p, \dot{e}_p \rangle + \mu\, k_2\, \eta_p\, \dot{\eta}_p \leq 0. \tag{4.9}$$

That is,

$$\langle \sigma + \mu\, H_\chi\, (\text{sym}\, \chi_p - e_p), \dot{e}_p \rangle - \mu\, k_2\, \eta_p\, \dot{\eta}_p \geq 0, \tag{4.10}$$

which can also be written in compact form as

$$\langle \Sigma_p, \dot{\Gamma}_p \rangle \geq 0 \tag{4.11}$$

where

$$\Sigma_p := (\Sigma_E, g) \quad \text{and} \quad \Gamma_p = (e_p, \eta_p) \tag{4.12}$$

with Σ_E being a symmetric Eshelby-type stress tensor and g being a thermodynamic force-type variable conjugate to $\dot{\eta}_p$ and defined as

$$\Sigma_E := \sigma + \mu\, H_\chi(\text{sym}\, \chi_p - e_p) = \sigma - \mu\, L_c^2\, \text{Curl Curl}\, \chi_p, \tag{4.13}$$

$$g := -\mu\, k_2\, \eta_p. \tag{4.14}$$

4.1.3. The flow rule

We consider a yield function defined by

$$\phi(\Sigma_p) := \|\text{dev}\, \Sigma_{\text{E}}\| + g - \sigma_0 \quad \text{for}\ \Sigma_p = (\Sigma_E, g). \tag{4.15}$$

So the set of admissible (elastic) generalized stresses is defined as

$$\mathscr{K} := \{\Sigma_p = (\Sigma_{\text{E}}, g) \mid \phi(\Sigma_p) \leq 0, g \leq 0\}. \tag{4.16}$$

The principle of maximum dissipation gives the normality law

$$\dot{\Gamma}_p \in N_{\mathscr{K}}(\Sigma_p), \tag{4.17}$$

where $N_{\mathscr{K}}(\Sigma_p)$ denotes the normal cone to $\mathscr{K}$ at Σ_p, which is the set of generalized strain rates $\dot{\Gamma}_p$ that satisfy

$$\langle \overline{\Sigma} - \Sigma_p, \dot{\Gamma}_p \rangle \leq 0 \quad \text{for all}\ \ \overline{\Sigma} \in \mathscr{K}. \tag{4.18}$$

Notice that $N_{\mathscr{K}} = \partial\chi_{\mathscr{K}}$ where $\chi_{\mathscr{K}}$ denotes the indicator function of the set $\mathscr{K}$ and $\partial\chi_{\mathscr{K}}$ denotes the subdifferential of the function $\chi_{\mathscr{K}}$.

Whenever the yield surface $\partial\mathscr{K}$ is smooth at Σ_p then

$$\dot{\Gamma}_p \in N_{\mathscr{K}}(\Sigma_p) \quad \Rightarrow \quad \exists \lambda \text{ such that } \dot{\varepsilon}_p = \lambda \frac{\operatorname{dev} \Sigma_E}{\|\operatorname{dev} \Sigma_E\|} \quad \text{and} \quad \dot{\eta}_p = \lambda = \|\dot{\varepsilon}_p\|$$

with the Karush-Kuhn Tucker conditions: $\lambda \geq 0$, $\phi(\Sigma_p) \leq 0$ and $\lambda\, \phi(\Sigma_p) = 0$.

Using convex analysis (Legendre-transformation) we find that

$$\underbrace{\dot{\Gamma}_p \in \partial \chi_{\mathscr{K}}(\Sigma_p)}_{\textbf{flow rule in its dual formulation}} \quad \Leftrightarrow \quad \underbrace{\Sigma_p \in \partial \chi^*_{\mathscr{K}}(\dot{\Gamma}_p)}_{\textbf{flow rule in its primal formulation}} \tag{4.19}$$

where $\chi^*_{\mathscr{K}}$ is the Fenchel-Legendre dual of the function $\chi_{\mathscr{K}}$ denoted in this context by $\mathscr{D}_{\text{iso}}$, the one-homogeneous dissipation function for rate-independent processes. That is, for every $\Gamma = (q, \beta)$,

$$\begin{aligned} \mathscr{D}_{\text{iso}}(\Gamma) &= \sup\{\langle \Sigma_p, \Gamma\rangle \mid \Sigma_p \in \mathscr{K}\} \\ &= \sup\{\langle \Sigma_E, q\rangle + g\beta \mid \phi(\Sigma_E, g) \leq 0, g \leq 0\} \\ &= \begin{cases} \sigma_0 \|q\| & \text{if } \|q\| \leq \beta, \\ \infty & \text{otherwise.} \end{cases} \end{aligned} \tag{4.20}$$

We get from the definition of the subdifferential $(\Sigma_p \in \partial \chi^*_{\mathscr{K}}(\dot{\Gamma}_p))$ that,

$$\mathscr{D}_{\text{iso}}(\Gamma) \geq \mathscr{D}_{\text{iso}}(\dot{\Gamma}_p) + \langle \Sigma_p, \Gamma - \dot{\Gamma}_p\rangle \quad \text{for any } \Gamma. \tag{4.21}$$

That is,

$$\mathscr{D}_{\text{iso}}(q, \beta) \geq \mathscr{D}_{\text{iso}}(\dot{\varepsilon}_p, \dot{\eta}_p) + \langle \Sigma_E, q - \dot{\varepsilon}_p\rangle + g(\beta - \dot{\eta}_p) \quad \text{for any } (q, \beta). \tag{4.22}$$

In the next sections, we present as in the case of single-crystal gradient plasticity, a complete mathematical analysis of the model including both strong and weak formulations as well as a corresponding existence result.

4.1.4. Strong formulation of the model

To summarize, we have obtained the following strong formulation for the microcurl model in the poycrystalline infinitesimal gradient plasticity setting with isotropic hardening. Given $f \in \mathrm{H}^1(0, T; L^2(\Omega, \mathbb{R}^3))$, the goal is to find:

(i) the displacement $u \in \mathrm{H}^1(0, T; H^1_0(\Omega, \Gamma_{\mathrm{D}}, \mathbb{R}^3))$,
(ii) the infinitesimal plastic strain $\varepsilon_p \in \mathrm{H}^1(0, T; L^2(\Omega, \mathrm{Sym}(3) \cap \mathfrak{sl}(3)))$, the infinitesimal micro-distortion χ_p with $\operatorname{sym} \chi_p \in \mathrm{H}^1(0, T; L^2(\Omega, \mathrm{Sym}(3) \cap \mathfrak{sl}(3)))$, $\operatorname{Curl} \chi_p \in \mathrm{H}^1(0, T; L^2(\Omega, \mathbb{R}^{3\times 3}))$ and $\operatorname{Curl}\operatorname{Curl} \chi_p \in \mathrm{H}^1(0, T; L^2(\Omega, \mathbb{R}^{3\times 3}))$

such that the content of Table 4 holds.

4.1.5. Weak formulation of the model

Assume that the problem in Section 4.1.4 has a solution

$$(u, \varepsilon_p, \chi_p, \eta_p).$$

Table 4
The microcurl model in polycrystalline gradient plasticity with isotropic hardening. The boundary condition on χ_p necessitates at least $\chi_p \in \mathrm{H}(\operatorname{Curl}; \Omega, \mathbb{R}^{3\times 3})$. This is proven to be the case in the next sections through a weak formulation of the model as a variational inequality.

Additive split of strain:	$\nabla u = e + p$, $\varepsilon_e = \operatorname{sym} e$, $\varepsilon_p = \operatorname{sym} p$
Equilibrium:	$\operatorname{Div} \sigma + f = 0$ with $\sigma = \mathbb{C}_{\text{iso}} \varepsilon_e = \mathbb{C}_{\text{iso}}(\operatorname{sym} \nabla u - \varepsilon_p)$
Microbalance:	$\mu\, L_c^2 \operatorname{Curl}\operatorname{Curl} \chi_p = -\mu\, H_\chi(\operatorname{sym} \chi_p - \varepsilon_p)$,
Free energy:	$\frac{1}{2}\langle \mathbb{C}.\varepsilon_e, \varepsilon_e\rangle + \frac{1}{2}\mu\, H_\chi \|\varepsilon_p - \operatorname{sym} \chi_p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\operatorname{Curl} \chi_p\|^2 + \frac{1}{2}\mu\, k_2 |\eta_p|^2$
Yield condition:	$\phi(\Sigma_E) := \|\operatorname{dev} \Sigma_E\| + g - \sigma_0 \leq 0$
where	$\Sigma_E := \sigma + \mu\, H_\chi(\operatorname{sym} \chi_p - \varepsilon_p)$, $g = -\mu\, k_2\, \eta_p$
Dissipation inequality:	$\langle \Sigma_E, \dot{\varepsilon}_p\rangle + g\dot{\eta}_p \geq 0$
Dissipation function:	$\mathscr{D}_{\text{iso}}(q, \beta) := \begin{cases} \sigma_0 \|q\| & \text{if } \|q\| \leq \beta, \\ \infty & \text{otherwise} \end{cases}$
Flow rule in primal form:	$(\Sigma_E, g) \in \partial \mathscr{D}_{\text{iso}}(\dot{\varepsilon}_p, \dot{\eta}_p)$
Flow rule in dual form:	$\dot{\varepsilon}_p = \lambda \frac{\operatorname{dev} \Sigma_E}{\|\operatorname{dev} \Sigma_E\|}$, $\quad \dot{\eta}_p = \lambda = \|\dot{\varepsilon}_p\|$
KKT conditions:	$\lambda \geq 0$, $\phi(\Sigma_E, g) \leq 0$, $\lambda\, \phi(\Sigma_E, g) = 0$
Boundary conditions for χ_p:	$\chi_p \times n = 0$ on Γ_{D}, $(\operatorname{Curl} \chi_p) \times n = 0$ on $\partial\Omega \setminus \Gamma_{\mathrm{D}}$
Function space for χ_p:	$\chi_p(t, \cdot) \in \mathrm{H}(\operatorname{Curl}; \Omega, \mathbb{R}^{3\times 3})$

Let $v \in H^1(\Omega, \mathbb{R}^3)$ with $v|_{\Gamma_D} = 0$. Multiply the equilibrium equation with $v - \dot{u}$ and integrate in space by parts and use the symmetry of σ and the elasticity relation to get

$$\int_\Omega \langle \mathbb{C}_{\text{iso}}(\text{sym}(\nabla u - \varepsilon_p)), \text{sym}\nabla v - \text{sym}\nabla \dot{u}\rangle dx = \int_\Omega f(v - \dot{u}) dx \tag{4.23}$$

Now, for any $X \in C^\infty(\overline{\Omega}, \mathfrak{sl}(3))$ such that $X \times n = 0$ on Γ_D we integrate (4.4) over Ω, integrate by parts the term with Curl Curl using the boundary conditions

$$(X - \dot{\chi}_p) \times n = 0 \text{ on } \Gamma_D, \quad \text{Curl } \chi_p \times n = 0 \text{ on } \partial\Omega \setminus \Gamma_D$$

and get

$$\int_\Omega \Big[\mu L_c^2 \langle \text{Curl } \chi_p, \text{Curl } X - \text{Curl } \dot{\chi}_p\rangle - \mu H_\chi \langle \varepsilon_p - \text{sym } \chi_p, \text{sym } X - \text{sym } \dot{\chi}_p\rangle\Big] dx = 0. \tag{4.24}$$

Moreover, for any $q \in C^\infty(\overline{\Omega}, \mathfrak{sl}(3))$ and any $\beta \in L^2(\Omega)$, we integrate (4.22) over Ω and get

$$\begin{aligned}\int_\Omega \mathscr{D}_{\text{iso}}(q, \beta) dx - \int_\Omega \mathscr{D}_{\text{iso}}(\dot{\varepsilon}_p, \dot{\eta}_p) dx - \int_\Omega \langle \mathbb{C}_{\text{iso}}(\text{sym}(\nabla u) - \varepsilon_p), q - \dot{\varepsilon}_p\rangle dx + \int_\Omega \Big[\mu H_\chi \langle \varepsilon_p - \text{sym } \chi_p, q - \dot{\varepsilon}_p\rangle \\ + \mu k_2 \eta_p(\beta - \dot{\eta}_p)\Big] dx \geq 0.\end{aligned} \tag{4.25}$$

Now adding up (4.23), (4.24) and (4.25) we get the following weak formulation of the problem in Section 4.1.4 in the form of a variational inequality:

$$\begin{aligned}&\int_\Omega \Big[\langle \mathbb{C}_{\text{iso}}(\text{sym}\nabla u - \varepsilon_p), (\text{sym}\nabla v - q) - (\text{sym}\nabla \dot{u} - \dot{\varepsilon}_p)\rangle + \mu L_c^2 \langle \text{Curl } \chi_p, \text{Curl } X - \text{Curl } \dot{\chi}_p\rangle + \mu H_\chi \langle \text{sym } \chi_p \\ &- \varepsilon_p, (\text{sym } X - q) - (\text{sym } \dot{\chi}_p - \dot{\varepsilon}_p)\rangle + \mu k_2 \eta_p(\beta - \dot{\eta}_p)\Big] dx + \int_\Omega \mathscr{D}_{\text{iso}}(q, \beta) dx - \int_\Omega \mathscr{D}_{\text{iso}}(\dot{\varepsilon}_p, \dot{\eta}_p) dx \\ &\geq \int_\Omega f(v - \dot{u}) dx\end{aligned} \tag{4.26}$$

4.1.6. Existence result for the weak formulation

As in the case of single-crystal gradient plasticity in Section 3.2.6, the existence result for the weak formulation (4.26) is obtained through the abstract machinery developed in Han and Reddy (2013) for mathematical problems in geometrically linear classical plasticity. To this aim, (4.26) is written as the variational inequality of the second kind: find $w = (u, \varepsilon_p, \chi_p, \eta_p) \in \text{H}^1(0, T; Z)$ such that $w(0) = 0$, $\dot{w}(t) \in W$ for a.e. $t \in [0, T]$ and

$$\boldsymbol{a}(\dot{w}, z - w) + j(z) - j(\dot{w}) \geq \langle \ell, z - \dot{w}\rangle \text{for every } z \in W \text{ and for a.e. } t \in [0, T], \tag{4.27}$$

where Z is a suitable Hilbert space and W is some closed, convex subset of Z to be constructed later,

$$\boldsymbol{a}(w, z) = \int_\Omega \Big[\langle \mathbb{C}_{\text{iso}}(\text{sym}\nabla u - \varepsilon_p), \text{sym}\nabla v - q\rangle + \mu L_c^2 \langle \text{Curl } \chi_p, \text{Curl } X\rangle + \mu H_\chi \langle \text{sym } \chi_p - \varepsilon_p, \text{sym } X - q\rangle + \mu k_2 \eta_p \beta\Big] dx, \tag{4.28}$$

$$j(z) = \int_\Omega \mathscr{D}_{\text{iso}}(q, \beta)\, dx\,, \tag{4.29}$$

$$\langle \ell, z\rangle = \int_{\Omega} f\, v\, dx\,, \tag{4.30}$$

for $w=(u,\varepsilon_p,\chi_p,\eta_p)$ and $z=(v,q,X,\beta)$ in Z.

The Hilbert space Z and the closed convex subset W are constructed in such a way that the functionals $\boldsymbol{a}$, j and ℓ satisfy the assumptions in the abstract result in Han and Reddy (2013), Theorem 6.19. The key issue here is the coercivity of the bilinear form $\boldsymbol{a}$ on the set W, that is, $a(z,z)\geq C\|z\|_Z^2$ for every $z\in$Z and for some $C>0$.

We let

$$\mathrm{V} := \mathrm{H}_0^1(\Omega,\Gamma_{\mathrm{D}},\mathbb{R}^3) = \{v\in \mathrm{H}^1(\Omega,\mathbb{R}^3)\,|\, v_{|\Gamma_{\mathrm{D}}}=0\}, \tag{4.31}$$

$$\mathrm{P} := \mathrm{L}^2(\Omega,\mathfrak{sl}(3)\cap \mathrm{Sym}(3)), \tag{4.32}$$

$$\mathrm{Q} := \mathrm{H}_0(\mathrm{Curl};\Omega,\Gamma,\mathfrak{sl}(3)), \tag{4.33}$$

$$\Lambda := L^2(\Omega), \tag{4.34}$$

$$\mathrm{Z} := \mathrm{V}\times \mathrm{P}\times \mathrm{Q}\times \Lambda, \tag{4.35}$$

$$\mathrm{W} := \{z=(v,q,X,\beta)\in\ \mathrm{Z}\ |\ \|q\|\leq \beta\}, \tag{4.36}$$

and define the norms

$$\begin{aligned} &\|v\|_V := \|\nabla v\|_{L^2},\quad \|q\|_P = \|q\|_{L^2},\quad \|X\|_Q := \|X\|_{\mathrm{H(Curl};\Omega)},\\ &\|z\|_Z^2 := \|v\|_V^2 + \|q\|_{L^2}^2 + \|X\|_Q^2 + \|\beta\|_{L^2}^2 \quad \text{for } z=(v,q,X,\beta)\in \mathrm{Z}. \end{aligned} \tag{4.37}$$

Let us show that the bilinear form $\boldsymbol{a}$ is coercive on W. Let therefore $z=(v,q,X,\beta)\in$W.

$$\begin{aligned} \boldsymbol{a}(z,z) &\geq m_0\|\mathrm{sym}\nabla v - q\|_{L^2}^2 (\text{from} (2.3)) + \mu H_\chi \|\mathrm{sym}\, X - q\|_{L^2}^2 + \mu L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2 + \mu k_2\|\beta\|_{L^2}^2\\ &= m_0\left[\|\mathrm{sym}\nabla v\|_{L^2}^2 + \|q\|_{L^2}^2 - 2\langle \mathrm{sym}\nabla v, q\rangle\right] + \mu H_\chi\left[\|\mathrm{sym}\, X\|_{L^2}^2 + \|q\|_{L^2}^2 - 2\langle \mathrm{sym}\, X, q\rangle\right] + \mu L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2 + \mu k_2\|\beta\|_{L^2}^2\\ &\geq m_0\left[\|\mathrm{sym}\nabla v\|_{L^2}^2 + \|q\|_{L^2}^2 - \theta\|\mathrm{sym}\nabla v\|_{L^2}^2 - \frac{1}{\theta}\|q\|_{L^2}^2\right] (\text{Young's inequality}) + \mu H_\chi\left[\|\mathrm{sym}\, X\|_{L^2}^2 + \|q\|_{L^2}^2 - \theta\|\mathrm{sym}\, X\|_{L^2}^2\right.\\ &\quad \left. -\frac{1}{\theta}\|q\|_{L^2}^2\right] (\text{Young's inequality}) + \mu L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2 + \frac{1}{2}\mu k_2\|\beta\|_{L^2}^2 + \frac{1}{2}\mu k_2\|q\|_{L^2}^2 \ (\text{using } \|q\|\leq\beta)\\ &= m_0(1-\theta)\|\mathrm{sym}\nabla v\|_{L^2}^2 + \left[(m_0+\mu H_\chi)\left(1-\frac{1}{\theta}\right) + \frac{1}{2}\mu k_2\right]\|q\|_{L^2}^2 + \mu H_\chi(1-\theta)\|\mathrm{sym}\, X\|_{L^2}^2 + \mu L_c^2\|\mathrm{Curl}\, X\|_{L^2}^2\\ &\quad + \frac{1}{2}\mu k_2\|\beta\|_{L^2}^2. \end{aligned} \tag{4.38}$$

So, since the hardening constant $k_2>0$, it is possible to choose θ such that

$$\frac{m_0+\mu H_\chi}{m_0+\mu H_\chi+\frac{1}{2}\mu k_2} < \theta < 1,$$

and using Korn's first inequality (see e.g. Neff, 2002) and the Korn-type inequality for incompatible tensor fields established in (Bauer et al., 2014, 2016; Neff et al., 2011, 2012a, 2012b, 2014b), namely

$$\|X\|_{L^2}^2 \leq C\left(\|\mathrm{sym}\, X\|_{L^2}^2 + \|\mathrm{Curl}\, X\|_{L^2}^2\right) \quad \forall X\in \mathrm{H}_0(\mathrm{Curl};\Omega,\Gamma_{\mathrm{D}},\mathbb{R}^{3\times 3}), \tag{4.39}$$

there exists some constant $C(m_0,\mu,H_\chi,k_2,L_c,\Omega)>0$ such that

$$a(z,z)\geq C\left[\|v\|_V^2 + \|q\|_{L^2}^2 + \|X\|_{\mathrm{H(Curl};\Omega)}^2 + \|\beta\|_{L^2}^2\right] = C\|z\|_Z^2 \quad \forall z=(v,q,X,\beta)\in \mathrm{W}. \tag{4.40}$$

This shows existence for our microcurl model in polycrystalline gradient plasticity with isotropic hardening.

Remark 4.1. Arguing as in Section 3.2.7, we get for any two solutions $(u_i, \varepsilon_{p\,i}, \chi_{p\,i}, \eta_{p\,i})$ with $i = 1,\ 2$ of (4.26) that

$$u_1 = u_2, \quad \varepsilon_{p_1} = \varepsilon_{p_2}, \quad \eta_{p_1} = \eta_{p_2}, \quad \operatorname{sym} \chi_{p_1} = \operatorname{sym} \chi_{p_2}, \quad \operatorname{Curl} \chi_{p_1} = \operatorname{Curl}_{p_2}$$

Now, using the Korn-type inequality for incompatible tensor fields established in Neff et al. (2011, 2012a, 2012b, 2014b) and applied to $\chi_{p\,1} - \chi_{p\,2}$, namely

$$\|\chi_{p_1} - \chi_{p_2}\|_{L^2}^2 \leq C\Big(\|\operatorname{sym}(\chi_{p_1} - \chi_{p_2})\|_{L^2}^2 + \|\operatorname{Curl}(\chi_{p_1} - \chi_{p_2})\|_{L^2}^2\Big), \tag{4.41}$$

we also get that $\chi_{p\,1} = \chi_{p\,2}$ and this show the uniqueness of the weak/strong solution.

4.2. The model with linear kinematical hardening

Here we consider the model where the isotropic hardening has been replaced with linear kinematical hardening. Here the free-energy is given by

$$\Psi(\nabla u, \varepsilon_p, \chi_p, \operatorname{Curl} \chi_p) := \underbrace{\Psi_e^{\operatorname{lin}}(\varepsilon_e)}_{\text{elastic energy}} + \underbrace{\Psi_{\operatorname{micro}}^{\operatorname{lin}}(\varepsilon_p, \chi_p)}_{\text{micro energy}} + \underbrace{\Psi_{\operatorname{curl}}^{\operatorname{lin}}(\operatorname{Curl} \chi_p)}_{\text{defect-like energy (GND)}} + \underbrace{\Psi_{\operatorname{kin}}^{\operatorname{lin}}(\varepsilon_p)}_{\text{hardening energy (SSD)}}, \tag{4.42}$$

where

$$\begin{aligned} \Psi_e^{\operatorname{lin}}(\varepsilon_e) &:= \frac{1}{2}\langle \varepsilon_e, \mathbb{C}_{\operatorname{iso}}\varepsilon_e\rangle = \frac{1}{2}\langle \operatorname{sym}\nabla u - \varepsilon_p, \mathbb{C}_{\operatorname{iso}}(\operatorname{sym}\nabla u - \varepsilon_p)\rangle, \\ \Psi_{\operatorname{micro}}^{\operatorname{lin}}(\varepsilon_p, \chi_p) &:= \frac{1}{2}\mu\, H_\chi \|\varepsilon_p - \operatorname{sym} \chi_p\|^2, \\ \Psi_{\operatorname{curl}}^{\operatorname{lin}}(\operatorname{Curl} \chi_p) &:= \frac{1}{2}\mu\, L_c^2 \|\operatorname{Curl} \chi_p\|^2, \quad \Psi_{\operatorname{kin}}^{\operatorname{lin}}(\varepsilon_p) := \frac{1}{2}\mu\, k_1 \|\varepsilon_p\|^2. \end{aligned} \tag{4.43}$$

The strong formulation of the model is presented in Table 5 while the weak formulation reads as

Table 5
The microcurl model in polycrystalline gradient plasticity with kinematical hardening. Also in this model, the boundary condition on $\chi_{\boldsymbol{p}}$ necessitates at least $\chi_{\boldsymbol{p}} \in \mathrm{H}(\operatorname{Curl}; \Omega, \mathbb{R}^{\mathbf{3\times 3}})$. Unlike the model with isotropic hardening for which uniqueness is obtained through the strong formulation, here we have uniqueness of the weak solution straight from the formulation as a variational inequality.

Additive split of strain:	$\nabla u = e + p$, $\varepsilon_e = \operatorname{sym} e$, $\varepsilon_p = \operatorname{sym} p$
Equilibrium:	$\operatorname{Div} \sigma + f = 0$ with $\sigma = \mathbb{C}_{\operatorname{iso}}\, \varepsilon_e = \mathbb{C}_{\operatorname{iso}}(\operatorname{sym}\nabla u - \varepsilon_p)$
Microbalance:	$\mu\, L_c^2 \operatorname{Curl} \operatorname{Curl} \chi_p = -\mu\, H_\chi(\operatorname{sym} \chi_p - \varepsilon_p)$,
Free energy:	$\frac{1}{2}\langle \mathbb{C}_{\operatorname{iso}}\varepsilon_e, \varepsilon_e\rangle + \frac{1}{2}\mu\, H_\chi \|\varepsilon_p - \operatorname{sym} \chi_p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\operatorname{Curl} \chi_p\|^2 + \frac{1}{2}\mu\, k_1 \|\operatorname{sym} p\|^2$
Yield condition:	$\phi(\Sigma_E) := \|\operatorname{dev} \Sigma_E\| - \sigma_0 \leq 0$
where	$\Sigma_E := \sigma + \Sigma_{\operatorname{micro}}^{\operatorname{lin}} + \Sigma_{\operatorname{kin}}^{\operatorname{lin}}$
with	$\Sigma_{\operatorname{micro}}^{\operatorname{lin}} = \mu\, H_\chi(\operatorname{sym} \chi_p - \varepsilon_p) = -\mu\, L_c^2 \operatorname{Curl} \operatorname{Curl} \chi_p$
	$\Sigma_{\operatorname{kin}}^{\operatorname{lin}} = -\mu\, k_1 \varepsilon_p$
Dissipation inequality:	$\int_\Omega \langle \Sigma_E, \dot{\varepsilon}_p\rangle dx \geq 0$
Dissipation function:	$\mathscr{D}_{\operatorname{kin}}(q) := \sigma_0 \|q\|$
Flow law in primal form:	$\Sigma_E \in \partial \mathscr{D}_{\operatorname{kin}}(\dot{\varepsilon}_p)$
Flow law in dual form:	$\dot{\varepsilon}_p = \lambda \frac{\operatorname{dev} \Sigma_E}{\|\operatorname{dev} \Sigma_E\|}$
KKT conditions:	$\lambda \geq 0$, $\phi(\Sigma_E) \leq 0$, $\lambda\, \phi(\Sigma_E) = 0$
Boundary conditions for χ_p:	$\chi_p \times n = 0$ on Γ_{D}, $(\operatorname{Curl} \chi_p) \times n = 0$ on $\partial\Omega \setminus \Gamma_{\mathrm{D}}$
Function space for χ_p:	$\chi_p(t, \cdot) \in \mathrm{H}(\operatorname{Curl}; \Omega, \mathbb{R}^{3\times 3})$

$$\int_\Omega \Big[\langle \mathbb{C}_{\rm iso}(\mathrm{sym}\nabla u - \varepsilon_p), (\mathrm{sym}\nabla v - q) - (\mathrm{sym}\nabla \dot{u} - \dot{\varepsilon}_p)\rangle + \mu\, L_c^2 \langle \mathrm{Curl}\, \chi_p, \mathrm{Curl}\, \mathrm{Q} - \mathrm{Curl}\, \dot{\chi}_p\rangle + \mu\, H_\chi \langle \mathrm{sym}\, \chi_p - \varepsilon_p, (\mathrm{sym}\, \mathrm{Q} - q) - (\mathrm{sym}\, \dot{\chi}_p - \dot{\varepsilon}_p)\rangle + \mu\, k_1 \langle \varepsilon_p\, q - \dot{\varepsilon}_p\rangle\Big]\, dx + \int_\Omega \mathscr{D}_{\rm kin}(q) dx - \int_\Omega \mathscr{D}_{\rm kin}(\dot{\varepsilon}_p) dx \geq \int_\Omega f(v - \dot{u}) dx. \tag{4.44}$$

That is, setting $\mathrm{Z} := \mathrm{V} \times \mathrm{P} \times \mathrm{Q}$ with V and Q defined in (4.31)–(4.33), $\mathrm{P} = L^2(\Omega, \mathrm{Sym}(3) \cap \mathfrak{sl}(3))$ and their norms in (4.37), we get the problem of the form: Find $w = (u, \varepsilon_p, \chi_p) \in \mathrm{H}^1(0, T; Z)$ such that $w(0) = 0$ and

$$\boldsymbol{a}(\dot{w}, z - w) + j(z) - j(\dot{w}) \geq \langle \ell, z - \dot{w}\rangle \text{for every } z \in \mathrm{Z} \text{ and for a.e. } t \in [0, T], \tag{4.45}$$

where

$$\boldsymbol{a}(w, z) = \int_\Omega \Big[\langle \mathbb{C}_{\rm iso}(\mathrm{sym}\nabla u - \varepsilon_p), \mathrm{sym}\nabla v - q\rangle + \mu\, L_c^2 \langle \mathrm{Curl}\, \chi_p, \mathrm{Curl}\, X\rangle + \mu\, H_\chi \langle \mathrm{sym}\, \chi_p - \varepsilon_p, \mathrm{sym}\, X - q\rangle + \mu\, k_1 \langle \varepsilon_p, q\rangle\Big]\, dx, \tag{4.46}$$

$$j(z) = \int_\Omega \mathscr{D}_{\rm kin}(q) dx, \tag{4.47}$$

$$\langle \ell, z\rangle = \int_\Omega f\, v\, dx, \tag{4.48}$$

for $w = (u, \varepsilon_p, \chi_p)$ and $z = (v, q, X)$ in Z.

The existence and uniqueness result for the problem in (4.45)–(4.48) is obtained from Han and Reddy (2013), Theorem 6.15 as the bilinear form $\boldsymbol{a}$ is Z-coercive (arguing as in (4.38)).

5. The relaxed linear micromorphic continuum

The relaxed micromorphic model is a very special subclass of the micromorphic model approach in which the extra dependence on gradients of the micro-distortion appears only through the Curl-operator. In the static and isotropic cases, the purely elastic model consists of a two-field minimization problem for the displacement $u : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$ and the non-symmetric micro-distortion tensor $\chi_p : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^{3\times 3}$ so that for

$$\begin{aligned} \mathscr{E}(u, \chi_p) := \int_\Omega \Big[& \mu_e \|\mathrm{sym}(\nabla u - \chi_p)\|^2 + \mu_c \|\mathrm{skew}(\nabla u - \chi_p)\|^2 + \frac{\lambda_e}{2} (\mathrm{tr}(\nabla u - \chi_p))^2 + \mu_{\rm micro} \|\mathrm{sym}\, \chi_p\|^2 \\ & + \frac{\lambda_{\rm micro}}{2} (\mathrm{tr}(\chi_p))^2 + \mu_e \frac{L_c^2}{2} \|\mathrm{Curl}\, \chi_p\|^2 \Big] dx, \end{aligned} \tag{5.1}$$

$$\mathscr{E}(u, \chi_p) \to \min \text{ w.r.t} (u,\ \chi_p) \tag{5.2}$$

subject to displacement boundary conditions $u|_{\Gamma_{\rm D}} = 0$ and the tangential boundary conditions $\chi_p \times n|_{\Gamma_{\rm D}} = 0$ (equivalent to $\chi_p \cdot \tau|_{\Gamma_{\rm D}} = 0$ for all vectors τ tangent to $\Gamma_{\rm D}$). Here, μ_e and λ_e with

$$\mu_e > 0 \quad \text{and} \quad 2\mu_e + 3\lambda_e > 0, \tag{5.3}$$

are new elastic material constants which are **not** the Lamé constants of linear elasticity. Well-posedness results in statics and dynamics have been obtained in Neff et al. (2014a, 2015), making crucial use of a recently established Korn's inequality for incompatible tensor fields (Neff et al., 2011, 2012a, 2012b, 2014b). The parameter $\mu_c \geq 0$ is called the Cosserat couple modulus and may be set to zero in this model.

Regarding the relation to the polycrystalline microcurl model (4.42)–(4.43), we see that in (5.1) the minimization variable χ_p is elastically coupled to the displacement gradient ∇u instead of being (penalty)-coupled to the plastic distortion p in the microcurl model (4.42)–(4.43).

In the single crystal microcurl model, the equation for the micro-distortion can be obtained from the one-field minimization problem

$$\int_\Omega \left[\frac{1}{2}\mu\, H_\chi \|p-\chi_p\|^2 + \frac{1}{2}\mu\, L_c^2 \|\mathrm{Curl}\,\chi_p\|^2\right] dx \to \min \chi_p \tag{5.4}$$

at given plastic distortion p.

Now, if we let $\mu_e,\ \mu_c,\ \lambda_e \to \infty$ ($\chi_p \to \nabla u$) then the static model turns indeed into a linear elastic model

$$\int_\Omega \left[\mu_\infty \|\mathrm{sym}\nabla u\|^2 + \frac{\lambda_\infty}{2}(\mathrm{tr}(\nabla u))^2\right] dx \to \min u, \tag{5.5}$$

where $\lambda_\infty,\ \mu_\infty$ can be determined analytically (Barbagallo et al., 2017).

The formulation (5.1) in the dynamic case has a number of distinguishing features. As it turns out, the so-called metamaterials with band-gaps at certain frequency ranges can be qualitatively and quantitatively described. For this, a nonzero Cosserat couple modulus $\mu_c > 0$ is mandatory. Materials that do not show band-gaps must be modelled with $\mu_c = 0$. Note that the formulation (5.1) contains as the special case $\mu_{\text{micro}},\ \lambda_{\text{micro}} \to \infty$ the well-known infinitesimal Cosserat model in which the additional field χ_p is restricted to be skew-symmetric (i.e., χ_p is set as $A \in \mathfrak{so}(3)$) and the elastic minimization problem reads

$$\int_\Omega \left[\mu\|\mathrm{sym}\nabla u\|^2 + \frac{\lambda}{2}(\mathrm{tr}(\nabla u))^2 + \mu_c\|\mathrm{skew}(\nabla u - A)\|^2 + \mu\frac{L_c^2}{2}\|\mathrm{Curl}\,A\|^2\right] dx \to \min(\mu, A), \tag{5.6}$$

see e.g. Barbagallo et al. (2017). The latter formulation has been coupled to perfect plasticity in an endevour to regularize ill-posedness of perfect plasticity, see e.g. Neff and Chełmiński (2007) and Neff et al. (2007).

6. Conclusion

Examples of finite element computations based on the microcurl single crystal models can be found in Cordero et al. (2013) where polycrystalline microstructures are discetized in order to account for grain size effects on the local stress and lattice curvatures fields inside the grains and on the overall Hall-Petch effect. Orowan-type size effects were addressed for laminate microstructures in Wulfinghof et al. (2015). It remains to implement the polycrystalline formulation proposed in the present work and to compare its response to that of polycrystalline aggregates using the single crystal model. In that way the new material parameters could be identified from this multiscale analysis. This would also help to decide between the two possible penalty couplings, namely

$$\underbrace{\frac{1}{2}\mu\, H_\chi \|p-\chi_p\|^2}_{\text{direct coupling}} \quad \text{versus} \quad \underbrace{\frac{1}{2}\mu\, H_\chi \|\mathrm{sym}(p-\chi_p)\|^2}_{\substack{\text{symmetric coupling}\\ \text{treated in this work}}}.$$

Mathematically, both formulations are well-posed, provided sufficient hardening is present. The direct coupling has the advantage of a clear penalty interpretation while the symmetric coupling does not see the plastic spin altogether, which may be advantageous from a modelling and implementational point of view.

The present mathematical analysis was performed within the infinitesimal framework. The reader is referred to Aslan et al. (2011) for a finite deformation formulation of the microcurl single crystal model that can be used for further applications involving significant lattice rotations and strains.

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