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NON-LOCAL CONTINUUM THERMODYNAMIC EXTENSIONS OF CRYSTAL PLASTICITY TO INCLUDE THE EFFECTS OF GEOMETRICALLY-NECESSARY DISLOCATIONS ON THE MATERIAL BEHAVIOUR

Abstract. The purpose of this work is the formulation of constitutive models for the inelastic material behaviour of single crystals and polycrystals in which geometrically-necessary dislocations (GNDs) may develop and influence this behaviour. To this end, we focus on the dependence of the development of such dislocations on the inhomogeneity of the inelastic deformation in the material. More precisely, in the crystal plasticity context, this is a relation between the density of GNDs and the inhomogeneity of inelastic deformation in glide systems. In this work, two models for GND density and its evolution, i.e., a glide-system-based model, and a continuum model, are formulated and investigated. As it turns out, the former of these is consistent with the original two-dimensional GND model of Ashby (1970), and the latter with the more recent model of Dai and Parks (1997). Since both models involve a dependence of the inelastic state of a material point on the (history of the) inhomogeneity of the glide-system inelastic deformation, their incorporation into crystal plasticity modeling necessarily implies a corresponding non-local generalization of this modeling. As it turns out, a natural quantity on which to base such a non-local continuum thermodynamic generalization, i.e., in the context of crystal plasticity, is the glide-system (scalar) slip deformation. In particular, this is accomplished here by treating each such slip deformation as either (1), a generalized "gradient" internal variable, or (2), as a scalar internal degree-of-freedom. Both of these approaches yield a corresponding generalized Ginzburg-Landau- or Cahn-Allen-type field relation for this scalar deformation determined in part by the dependence of the free energy on the dislocation state in the material. In the last part of the work, attention is focused on specific models for the free energy and its dependence on this state. After summarising and briefly discussing the initial-boundary-value problem resulting from the current approach as well as its algorithmic form suitable for numerical implementation, the work ends with a discussion of additional aspects of the formulation, and in particular the connection of the approach to GND modeling taken here with other approaches.

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1. Introduction

Standard micromechanical modeling of the inelastic material behaviour of metallic single crystals and polycrystals (e.g., Hill and Rice, 1972; Asaro, 1983; Cuitiño and Ortiz, 1992) is commonly based on the premise that resistance to glide is due mainly to the random trapping of mobile dislocations during locally homogeneous deformation. Such trapped dislocation are commonly referred to as statistically-stored dislocations (SSDs), and act as obstacles to further dislocation motion, resulting in hardening. As anticipated in the work of Nye (1953) and Kröner (1960), and discussed by Ashby (1970), an additional contribution to the density of immobile dislocations and so to hardening can arise when the continuum lengthscale (e.g., grain size) approaches that of the dominant microstructural features (e.g., mean spacing between precipitates relative to the precipitate size, or mean spacing between glide planes). Indeed, in this case, the resulting deformation incompatibility between, e.g., "hard" inclusions and a "soft" matrix, is accomodated by the development of so-called geometrically-necessary dislocations (GNDs). Experimentally-observed effects in a large class of materials such as increasing material hardening with decreasing (grain) size (i.e., the Hall-Petch effect) are commonly associated with the development of such GNDs.

These and other experimental results have motivated a number of workers over the last few years to formulate various extensions (e.g., based on strain-gradients: Fleck and Hutchinson, 1993, 1997) to existing local models for phenomenological plasticity, some of which have been applied to crystal plasticity (e.g., the strain-gradient-based approach: Shu and Fleck, 1999; Cosserat-based approach: Forest et al., 1997) as well. Various recent efforts in this direction based on dislocation concepts, and in particular on the idea of Nye (1953) that the incompatibility of local inelastic deformation represents a continuum measure of dislocation density (see also Kröner, 1960; Mura, 1987), include Steinmann (1996), Dai and Parks (1997), Shizawa and Zbib (1999), Menzel and Steinmann (2000), Acharya and Bassani (2000), and most recently Cermelli and Gurtin (2001). In addition, the recent work of Ortiz and Repetto (1999) and Ortiz et al. (2000) on dislocation substructures in ductile single crystals demonstrates the fundamental connection between the incompatibility of the local inelastic deformation and the lengthscale of dislocation microstructures in FCC single crystals. In particular, the approaches of Dai and Parks (1997), Shizawa and Zbib (1999), and Archaya and Bassani (2000) are geared solely to the modeling of additional hardening due to GNDs and involve no additional field relations or boundary conditions. For example, the approach of Dai and Parks (1997) was used by Busso et al. (2000) to model additional hardening in two-phase nickel superalloys, and that of Archaya and Bassani (2000) by Archaya and Beaudoni (2000) to model grain-size effects in FCC and BCC polycrystals up to moderate strains. Except for the works of Acharya and Bassani (2000) and Cermelli and Gurtin (2001), which are restricted to kinematics, all of these presume directly or indirectly a particular dependence of the (free) energy and/or other dependent constitutive quantities (e.g., yield stress) on the gradients of inelastic state variables, and in particular on that of the local inelastic deformation, i.e., that determine its incompatibility. Yet more general formulations of crystal plasticity involving a (general) dependence of the free energy on the gradient of the local inelastic deformation can be found in, e.g., Naghdi and Srinivasa (1993, 1994), Le and Stumpf (1996), or in Gurtin (2000).

From the constitutive point of view, such experimental and modeling work clearly demonstrates the need to account for the dependence of the constitutive relations, and so material behaviour, on the inhomogeneity or "non-locality" of the internal fields as expressed by their gradients. In the phenomenological or continuum field context, such non-locality of the material behaviour is, or can be, accounted for in a number of existing approaches (e.g., Maugin, 1980;

Capriz, 1989; Maugin, 1990; Fried and Gurtin, 1993, 1994; Gurtin, 1995; Fried, 1996; Valanis, 1996, 1998) for broad classes of materials. It is not the purpose of the current work to compare and contrast any of these with each other in detail (in this regard, see, e.g., Maugin and Muschik, 1994; Svendsen, 1999); rather, we wish to apply two of them to formulate continuum thermodynamic models for crystal plasticity in which gradients of the inelastic fields in question influence the material behaviour. To this end, we must first identify the relevant internal fields. On the basis of the standard crystal plasticity constitutive relation for the local inelastic deformation $\boldsymbol{F}_{\mathrm{P}}$, a natural choice for the principal inelastic fields of the formulation is the set of glide-system deformations. In contrast, Le and Stumpf (1996) worked in their variational formulation directly with $\boldsymbol{F}_{\mathrm{P}}$, and Gurtin (2000) in his formulation based on configurational forces with the set of glide-system slip rates. In both of these works, a principal result takes the form of an extended or generalized Euler-Lagrange-, Ginzburg-Landau- or Cahn-Allen-type field relation for the respective principal inelastic fields. Generalized forms of such field relations for the glide-system deformations are obtained in the current work by modeling them in two ways. In the simplest approach, these are modeled as "generalized" internal variables (GIVs) via a generalization of the approach of Maugin (1990) to the modeling of the entropy flux. Alternatively, and more generally, these are modeled here as internal degrees-of-freedom (DOFs) via the approach of Capriz (1989) in the extended form discussed by Svendsen (2001a). In addition, as shown here, these formulations are general enough to incorporate in particular a number of models for GNDs (e.g., Ashby, 1970; Dai and Parks, 1997) and so provide a thermodynamic framework for extended non-local crystal plasticity modeling including the effects of GNDs on the material behaviour.

After some mathematical preliminaries (§2), the paper begins (§3) with a brief discussion and formulation of basic kinematic and constitutive issues and relations relevant to the continuum thermodynamic approach to crystal plasticity taken in this work. In particular, as mentioned above, the standard constitutive form for $\boldsymbol{F}_{\mathrm{P}}$ in crystal plasticity determines the glide-system slip deformations ("slips") as principal constitutive unknowns here. Having then established the corresponding constitutive class for crystal plasticity, we turn next to the thermodynamic field formulation and analysis (§§4-5), depending on whether the glide-system slips are modeled as generalized internal variables (GIVs) (§4), or as internal degrees-of-freedom (DOFs) (§5). Next, attention is turned to the formulation of two (constitutive) classes of GND models (§6), yielding in particular expressions for the glide-system effective (surface) density of GNDs. The first class of such models is based on the incompatibility of glide-system local deformation. To this class belong for example the original model of Ashby (1970) and the recent dislocation density tensor of Shizawa and Zbib (1999). The second is based on the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ and is consistent with the model of Dai and Parks (1997). With such models in hand, the possible dependence of the free energy on quantities characterising the dislocation state of the material (e.g., dislocation densities) and the corresponding consequences for the formulation are investigated (§7). Beyond the GND models formulated here, examples are also given of existing SSD models which can be incorporated into models for the free energy, and so into the current approach. After discussing simplifications arising in the formulation for the case of small deformation (§8), as well as the corresponding algorithmic form, the paper ends (§9) with a discussion of additional general aspects of the current approach and a comparison with other related work.

2. Mathematical preliminaries

If W and Z represent two finite-dimensional linear spaces, let $\mathrm{Lin}(W, Z)$ represent the set of all linear mappings from W to Z. If W and Z are inner product spaces, the inner products on W and Z induce the transpose $\mathcal{A}^{\mathrm{T}} \in \mathrm{Lin}(Z, W)$ of any $\mathcal{A} \in \mathrm{Lin}(W, Z)$, as well as the inner product $\mathcal{A}\cdot\mathcal{B} := \mathrm{tr}_W(\mathcal{A}^{\mathrm{T}}\mathcal{B}) = \mathrm{tr}_Z(\mathcal{A}\mathcal{B}^{\mathrm{T}})$ on $\mathrm{Lin}(W, Z)$ for all $\mathcal{A}, \mathcal{B} \in \mathrm{Lin}(W, Z)$. The main linear space of interest in this work is of course three-dimensional Euclidean vector space V. Let $\mathrm{Lin}(V, V)$ represent the set of all linear mappings of V into itself (i.e., second-order Euclidean tensors). Elements of V and $\mathrm{Lin}(V, V)$, or mappings taking values in these spaces, are denoted here as usual by bold-face, lower-case $\boldsymbol{a}, \ldots$ and upper-case $\boldsymbol{A}, \ldots$, italic letters, respectively. In particular, $\boldsymbol{I} \in \mathrm{Lin}(V, V)$ represents the second-order identity tensor. As usual, the tensor product $\boldsymbol{a} \otimes \boldsymbol{b}$ of any two $\boldsymbol{a}, \boldsymbol{b} \in V$ can be interpreted as an element $\boldsymbol{a} \otimes \boldsymbol{b} \in \mathrm{Lin}(V, V)$ of $\mathrm{Lin}(V, V)$ via $(\boldsymbol{a} \otimes \boldsymbol{b})\boldsymbol{c} := (\boldsymbol{b}\cdot\boldsymbol{c})\boldsymbol{a}$ for all $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in V$. Let $\mathrm{sym}(\boldsymbol{A}) := \frac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^{\mathrm{T}})$ and $\mathrm{skw}(\boldsymbol{A}) := \frac{1}{2}(\boldsymbol{A} - \boldsymbol{A}^{\mathrm{T}})$ represent the symmetric and skew-symmetric parts, respectively, of any $\boldsymbol{A} \in \mathrm{Lin}(V, V)$. The axial vector $\mathrm{axi}(\boldsymbol{W}) \in V$ of any skew tensor $\boldsymbol{W} \in \mathrm{Lin}(V, V)$ is defined by $\mathrm{axi}(\boldsymbol{W}) \times \boldsymbol{a} := \boldsymbol{W}\boldsymbol{a}$. Let $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in V$ be constant vectors in what follows.

Turning next to field relations, the definition

$$\mathrm{curl}\,\boldsymbol{u} := 2\,\mathrm{axi}(\mathrm{skw}(\nabla\boldsymbol{u})) \tag{1}$$

for the curl of a differentiable Euclidean vector field $\boldsymbol{u}$ is employed in this work, ∇ being the standard Euclidean gradient operator. In particular, (1) and the basic result

$$\nabla(f\boldsymbol{u}) = \boldsymbol{u} \otimes \nabla f + f(\nabla\boldsymbol{u}) \tag{2}$$

for all differentiable functions f and vector fields $\boldsymbol{u}$ yield the identity

$$\mathrm{curl}\,(f\boldsymbol{u}) = \nabla f \times \boldsymbol{u} + f(\mathrm{curl}\,\boldsymbol{u}) \quad . \tag{3}$$

In addition, (1) yields the identity

$$\mathrm{curl}\,\boldsymbol{u}\cdot\boldsymbol{a}\times\boldsymbol{b} = \nabla_{\boldsymbol{a}}\boldsymbol{u}\cdot\boldsymbol{b} - \nabla_{\boldsymbol{b}}\boldsymbol{u}\cdot\boldsymbol{a} \tag{4}$$

for $\mathrm{curl}\,\boldsymbol{u}$ in terms of the directional derivative

$$\nabla_{\boldsymbol{a}}\boldsymbol{u} := (\nabla\boldsymbol{u})\boldsymbol{a} \tag{5}$$

of $\boldsymbol{u}$ in the direction $\boldsymbol{a} \in V$. Turning next to second-order tensor fields, we work here with the definition*

$$(\mathrm{curl}\,\boldsymbol{T})^{\mathrm{T}}\boldsymbol{a} := \mathrm{curl}\,(\boldsymbol{T}^{\mathrm{T}}\boldsymbol{a}) \tag{6}$$

for the curl of a differentiable second-order Euclidean tensor field $\boldsymbol{T}$ as a second-order tensor field. From (3) and (6) follows in particular the identity

$$\mathrm{curl}\,(f\boldsymbol{T}) = \boldsymbol{T}(\boldsymbol{I} \times \nabla f) + f(\mathrm{curl}\,\boldsymbol{T}) \tag{7}$$

for all differentiable f and $\boldsymbol{T}$, where $(\boldsymbol{I} \times \boldsymbol{a})\boldsymbol{b} := \boldsymbol{b} \times \boldsymbol{a}$. Note that $(\boldsymbol{I} \times \boldsymbol{a})^{\mathrm{T}} = \boldsymbol{a} \times \boldsymbol{I}$ with $(\boldsymbol{a} \times \boldsymbol{I})\boldsymbol{b} := \boldsymbol{a} \times \boldsymbol{b}$. Likewise, (1) and (6) yield the identity

$$(\mathrm{curl}\,\boldsymbol{T})(\boldsymbol{a} \times \boldsymbol{b}) := (\nabla_{\boldsymbol{a}}\boldsymbol{T})\boldsymbol{b} - (\nabla_{\boldsymbol{b}}\boldsymbol{T})\boldsymbol{a} \tag{8}$$

for $\mathrm{curl}\,\boldsymbol{T}$ in terms of the directional derivative

$$\nabla_{\boldsymbol{a}}\boldsymbol{T}(\nabla\boldsymbol{T})\boldsymbol{a}$$

*This is of course a matter of convention. Indeed, in contrast to (6), Cermelli and Gurtin (2001) define $(\mathrm{curl}\,\boldsymbol{T})\boldsymbol{a} := \mathrm{curl}\,(\boldsymbol{T}^{\mathrm{T}}\boldsymbol{a})$.

of $\boldsymbol{T}$ in the direction $\boldsymbol{a} \in V$. Here, $\nabla\boldsymbol{T}$ represents a third-order Euclidean tensor field. Let $\boldsymbol{H}$ be a differentiable invertible tensor field. From (8) and the identity

$$\boldsymbol{A}^{\mathrm{T}}(\boldsymbol{A}\boldsymbol{b} \times \boldsymbol{A}\boldsymbol{c}) = \det(\boldsymbol{A})\,(\boldsymbol{b} \times \boldsymbol{c}) \tag{9}$$

for any second-order tensor $\boldsymbol{A} \in \mathrm{Lin}(V, V)$, we obtain

$$\mathrm{curl}\,(\boldsymbol{T}\boldsymbol{H}) = \det(\boldsymbol{H})\,(\mathrm{curl}^{\boldsymbol{H}}\boldsymbol{T})\boldsymbol{H}^{-\mathrm{T}} + \boldsymbol{T}\,(\mathrm{curl}\,\boldsymbol{H}) \tag{10}$$

for the curl of the product of two second-order tensor fields. Here, $\mathrm{curl}^{\boldsymbol{H}}$ represents the curl operator induced by the Koszul connection $\nabla^{\boldsymbol{H}}$ induced in turn by the invertible tensor field $\boldsymbol{H}$, i.e.,

$$\nabla^{\boldsymbol{H}}\boldsymbol{T} := (\nabla\boldsymbol{T})\boldsymbol{H}^{-1} \quad . \tag{11}$$

The corresponding curl operation then is defined in an analogous fashion to the standard form (8) relative to ∇.

Third-order tensors such as $\nabla\boldsymbol{T}$ are denoted in general in this work by A, B, ... and interpreted as elements of either $\mathrm{Lin}(V, \mathrm{Lin}(V, V))$ or $\mathrm{Lin}(\mathrm{Lin}(V, V), V)$. Note that any third-order tensor A induces one A^{S} defined by

$$(\mathsf{A}^{\mathrm{S}}\boldsymbol{b})\boldsymbol{c} := (\mathsf{A}\boldsymbol{c})\boldsymbol{b} \quad . \tag{12}$$

In particular, this induces the split

$$\mathsf{A} = \mathrm{sym}_{\mathrm{S}}(\mathsf{A}) + \mathrm{skw}_{\mathrm{S}}(\mathsf{A}) \tag{13}$$

of any third-order tensor A into "symmetric"

$$\mathrm{sym}_{\mathrm{S}}(\mathsf{A}) := \tfrac{1}{2}(\mathsf{A} + \mathsf{A}^{\mathrm{S}}) \tag{14}$$

and "skew-symmetric"

$$\mathrm{skw}_{\mathrm{S}}(\mathsf{A}) := \tfrac{1}{2}(\mathsf{A} - \mathsf{A}^{\mathrm{S}}) \tag{15}$$

parts. In addition, the latter of these induces the linear mapping

$$\mathrm{axi}_{\mathrm{S}} : \mathrm{Lin}(V, \mathrm{Lin}(V, V)) \longrightarrow \mathrm{Lin}(V, V) \quad | \quad \mathsf{A} \longmapsto \boldsymbol{A} = \mathrm{axi}_{\mathrm{S}}(\mathsf{A}) \tag{16}$$

defined by

$$\mathrm{axi}_{\mathrm{S}}(\mathsf{A})(\boldsymbol{b} \times \boldsymbol{c}) := 2\,(\mathrm{skw}_{\mathrm{S}}(\mathsf{A})\boldsymbol{b})\boldsymbol{c} = (\mathsf{A}\boldsymbol{b})\boldsymbol{c} - (\mathsf{A}\boldsymbol{c})\boldsymbol{b} \quad . \tag{17}$$

With the help of (12)–(17), one obtains in particular the compact form

$$\mathrm{curl}\,\boldsymbol{T} = \mathrm{axi}_{\mathrm{S}}(\nabla\boldsymbol{T}) \tag{18}$$

for the curl of a differentiable second-order tensor field $\boldsymbol{T}$ as a function of its gradient $\nabla\boldsymbol{T}$ from (8). The transpose $\mathsf{A}^{\mathrm{T}} \in \mathrm{Lin}(\mathrm{Lin}(V, V), V)$ of any third-order tensor $\mathsf{A} \in \mathrm{Lin}(V, \mathrm{Lin}(V, V))$ is defined here via $\mathsf{A}^{\mathrm{T}}\boldsymbol{B} \cdot \boldsymbol{c} = \boldsymbol{B} \cdot \mathsf{A}\boldsymbol{c}$.

Finally, for notational simplicity, it proves advantageous to abuse notation in this work and denote certain mappings and their values by the same symbol. Other notations and mathematical concepts will be introduced as they arise in what follows.

3. Basic kinematic, constitutive and balance relations

Let B represent a material body, $p \in B$ a material point of this body, and E Euclidean point space with translation vector space V. A motion of the body with respect to E in some time interval $I \subset \mathbb{R}$ takes as usual the form

$$\boldsymbol{x} = \xi(t, p)$$

relating each p to its (current) time $t \in I$ position $\boldsymbol{x} \in E$ in E. On this basis, $\dot{\xi}$ represents the material velocity, and

$$\boldsymbol{F}_\kappa(t, p) := (\nabla^\kappa \xi)(t, p) \in \mathrm{Lin}^+(V, V) \tag{19}$$

the deformation gradient relative to the (global) reference placement κ of B into E. Here, we are using the notation

$$\nabla^\kappa \xi := \kappa^*(\nabla(\kappa_* \xi))$$

for the gradient of ξ with respect to κ in terms of push-forward and pull-back, where $(\kappa_*\xi)(t, \boldsymbol{r}_\kappa) := \xi(t, \kappa^{-1}(\boldsymbol{r}_\kappa))$ for push-forward by κ, with $\boldsymbol{r}_\kappa = \kappa(p)$, and similarly for κ^*. Like ξ, $\dot{\xi}$ and $\boldsymbol{F}_\kappa$, all fields to follow are represented here as time-dependent fields on B. And analogous to that of ξ in (19), the gradients of these fields are all defined relative to κ. More precisely, these are defined at each $p \in B$ relative to a corresponding local reference placement† at each $p \in B$, i.e., an equivalence class of global placements κ having the same gradient at p. Since κ and the corresponding local reference placement at each $p \in B$ is arbitrary here, and the dependence of $\boldsymbol{F}_\kappa$ and the gradients of other fields, as well as that of the constitutive relations to follow, on κ does not play a direct role in the formulation in this work, we suppress it in the notation for simplicity.

In the case of phenomenological crystal plasticity, any material point $p \in B$ is endowed with a "microstructure" in the form of a set of n glide systems. The geometry and orientation of each such glide system is described as usual by an orthonormal basis $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$ $(\mathfrak{a} = 1, \ldots, n)$. Here, $\boldsymbol{s}_\mathfrak{a}$ represents the direction of glide in the plane, $\boldsymbol{n}_\mathfrak{a}$ the glide-plane normal, and $\boldsymbol{t}_\mathfrak{a} := \boldsymbol{s}_\mathfrak{a} \times \boldsymbol{n}_\mathfrak{a}$ the direction transverse to $\boldsymbol{s}_\mathfrak{a}$ in the glide plane. Since we neglect in this work the effects of any processes involving a change in or evolution of either the glide direction $\boldsymbol{s}_\mathfrak{a}$ or the glide-system orientation $\boldsymbol{n}_\mathfrak{a}$ (e.g., texture development), these referential unit vectors, and so $\boldsymbol{t}_\mathfrak{a}$ as well, are assumed constant with respect to the reference placement. With respect to the glide-system geometry, then, the (local) deformation $\boldsymbol{F}_\mathfrak{a}$ of each glide system takes the form of a simple shear‡

$$\boldsymbol{F}_\mathfrak{a} = \boldsymbol{I} + \gamma_\mathfrak{a}\, \boldsymbol{s}_\mathfrak{a} \otimes \boldsymbol{n}_\mathfrak{a} \quad , \tag{20}$$

$\gamma_\mathfrak{a}$ being its magnitude in the direction $\boldsymbol{s}_\mathfrak{a}$ of shear. For simplicity, we refer to each $\gamma_\mathfrak{a}$ as the (scalar) glide-system slip (deformation). The orthogonality of $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$ implies $\boldsymbol{F}_\mathfrak{a}^{\mathrm{T}} \boldsymbol{n}_\mathfrak{a} = \boldsymbol{n}_\mathfrak{a}$ and $\boldsymbol{F}_\mathfrak{a}\, \boldsymbol{s}_\mathfrak{a} = \boldsymbol{s}_\mathfrak{a}$, as well as $\gamma_\mathfrak{a} = \boldsymbol{s}_\mathfrak{a} \cdot \boldsymbol{F}_\mathfrak{a}\, \boldsymbol{n}_\mathfrak{a}$. In addition,

$$\dot{\boldsymbol{F}}_\mathfrak{a} = \boldsymbol{s}_\mathfrak{a} \otimes \boldsymbol{n}_\mathfrak{a}\, \dot{\gamma}_\mathfrak{a} =: \boldsymbol{L}_\mathfrak{a} \boldsymbol{F}_\mathfrak{a} \tag{21}$$

follows from (20). As such, the evolution of the glide-system deformation tensor $\boldsymbol{F}_\mathfrak{a}$ is determined completely by that of the corresponding scalar slip $\gamma_\mathfrak{a}$.

†Refered to by Noll (1967) as local reference configuration of $p \in B$ in E.

‡As discussed in §6, like $\boldsymbol{F}_\mathrm{P}$, and unlike $\boldsymbol{F}$, $\boldsymbol{F}_\mathfrak{a}$ is in general not compatible.

From a phenomenological point of view, the basic local inelastic deformation at each material point in the material body in question is represented by an invertible second-order tensor field $\boldsymbol{F}_{\mathrm{P}}$ on $I \times B$. The evolution of $\boldsymbol{F}_{\mathrm{P}}$ is given by the standard form

$$\dot{\boldsymbol{F}}_{\mathrm{P}} = \boldsymbol{L}_{\mathrm{P}} \boldsymbol{F}_{\mathrm{P}} \tag{22}$$

in terms of the plastic velocity "gradient" $\boldsymbol{L}_{\mathrm{P}}$. The connection to crystal plasticity is then obtained via the *constitutive* assumption

$$\boldsymbol{L}_{\mathrm{P}} \mathrel{\widehat{=}} \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{L}_{\mathfrak{a}} = \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}\, \dot{\gamma}_{\mathfrak{a}} \tag{23}$$

for $\boldsymbol{L}_{\mathrm{P}}$ via (21), where $m \leq n$ represents the set[§] of *active* glide-systems, i.e., those for which $\dot{\gamma}_{\mathfrak{a}} \neq 0$. Combining this last constitutive relation with (22) then yields the basic constitutive expression

$$\dot{\boldsymbol{F}}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{L}_{\mathfrak{a}}\, \boldsymbol{F}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{m} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}) \boldsymbol{F}_{\mathrm{P}}\, \dot{\gamma}_{\mathfrak{a}} \tag{24}$$

for the evolution of $\boldsymbol{F}_{\mathrm{P}}$. In turn, this basic constitutive relation implies that

$$\dot{\overline{\nabla \boldsymbol{F}_{\mathrm{P}}}} = \sum\nolimits_{\mathfrak{a}=1}^{m} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})(\nabla \boldsymbol{F}_{\mathrm{P}})\, \dot{\gamma}_{\mathfrak{a}} + (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}) \boldsymbol{F}_{\mathrm{P}} \otimes \nabla \dot{\gamma}_{\mathfrak{a}} \tag{25}$$

for the evolution of $\nabla \boldsymbol{F}_{\mathrm{P}}$, and so that

$$\dot{\overline{\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}}} = \sum\nolimits_{\mathfrak{a}=1}^{m} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})(\operatorname{curl} \boldsymbol{F}_{\mathrm{P}})\, \dot{\gamma}_{\mathfrak{a}} + \boldsymbol{s}_{\mathfrak{a}} \otimes (\nabla \dot{\gamma}_{\mathfrak{a}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}) \tag{26}$$

for the evolution of $\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}$ via (7) and (8). On this basis, the evolution relation for $\boldsymbol{F}_{\mathrm{P}}$ is *linear* in the set $\dot{\gamma} := (\dot{\gamma}_1, \ldots, \dot{\gamma}_m)$ of active glide-system slip rates. Similarly, the evolution relations for $\nabla \boldsymbol{F}_{\mathrm{P}}$ and $\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}$ are *linear* in $\dot{\gamma}$ and $\nabla \dot{\gamma}$. Generalizing the case of $\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}$ slightly, which represents one such measure, the dislocation state in the material is modeled phenomenologically in this work via a general inelastic state/dislocation measure α whose evolution is assumed to depend *quasi-linearly* on $\dot{\gamma}$ and $\nabla \dot{\gamma}$, i.e.,

$$\dot{\alpha} = \mathcal{K}\, \dot{\gamma} + \mathcal{J}\, \nabla \dot{\gamma} \tag{27}$$

in terms of the dependent constitutive quantities $\mathcal{K}$ and $\mathcal{J}$. In particular, on the basis of (24), $\boldsymbol{F}_{\mathrm{P}}$ is considered here to be an element of α. In turn, the dependence of this evolution relation on $\nabla \dot{\gamma}$ requires that we model the γ as time-dependent *fields* on B. As such, in the current thermomechanical context, the absolute temperature θ, the motion ξ, and the set γ of glide-system slips, represent the principal time-dependent fields, $\boldsymbol{F}_{\mathrm{P}}$ and α being determined constitutively by the history of γ and $\nabla \dot{\gamma}$ via (24) and (27), respectively. On the basis of determinism, local action, and short-term mechanical memory, then, the material behaviour of a given material point $p \in B$ is described by the general material frame-indifferent constitutive form

$$\mathfrak{R} = \mathfrak{R}(\theta, \boldsymbol{C}, \alpha, \nabla \theta, \dot{\gamma}, \nabla \dot{\gamma}, p) \tag{28}$$

for all dependent constitutive quantities (e.g., stress), where $\boldsymbol{C} = \boldsymbol{F}^{\mathrm{T}} \boldsymbol{F}$ represents the right Cauchy-Green deformation as usual. In particular, since the motion ξ, as well as the material

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[§] In standard crystal plasticity models, the number m of active glide system is determined among other things by the glide-system "flow rule," loading conditions, and crystal orientation. As such, it is constitutive in nature, and in general variable.

velocity $\dot{\xi}$, are not Euclidean frame-indifferent, $\mathfrak{R}$ is independent of these to satisfy material frame-indifference. As such, (28) represents the basic reduced constitutive form of the constitutive class of interest for the continuum thermodynamic formulation of crystal plasticity to follow. Because it plays no direct role in the formulation, the dependence of the constitutive relations on $p \in B$ is suppressed in the notation until needed.

The derivation of balance and field relations relative to the given reference configuration of B is based in this work on the local forms for total energy and entropy balance, i.e.,

$$\begin{aligned} \dot{e} &= \operatorname{div} \boldsymbol{h} + s \ , \\ \dot{\eta} &= \pi - \operatorname{div} \phi + \sigma \ , \end{aligned} \tag{29}$$

respectively. Here, e represents the total energy density, $\boldsymbol{h}$ its flux density, and s its supply rate density. Likewise, π, ϕ, and σ represent the production rate, flux, and supply rate, densities, respectively, of entropy, with density η. In particular, the mechanical balance relations follow from $(29)_1$ via its invariance with respect to Euclidean observer. And as usual, the thermodynamic analysis is based on $(29)_2$; in addition, it yields a field relation for the temperature, as will be seen in what follows.

This completes the synopsis of the basic relations required for the sequel. Next, we turn to the formulation of field relations and the thermodynamic analysis for the constitutive class determined by the form (28).

4. Generalized internal variable model for glide-system slips

The modeling of the γ as generalized internal variables (GIVs) is based in particular on the standard continuum forms

$$\begin{aligned} e &= \varepsilon &+& \tfrac{1}{2}\varrho\, \dot{\xi} \cdot \dot{\xi} \ , \\ \boldsymbol{h} &= -\boldsymbol{q} &+& \boldsymbol{P}^{\mathrm{T}} \dot{\xi} \ , \\ s &= r &+& \boldsymbol{f} \cdot \dot{\xi} \ , \end{aligned} \tag{30}$$

for total energy density e, total energy flux density $\boldsymbol{h}$, and total energy supply rate density s, respectively, hold. Here, ϱ represents the referential mass density, $\boldsymbol{P}$ the first Piola-Kirchhoff stress tensor, and $\boldsymbol{f}$ the momentum supply rate density. Further, ε represents the internal energy density, and $\boldsymbol{q}$ the heat flux density. As in the standard continuum case, $\boldsymbol{P}$, ε, $\boldsymbol{q}$, η and ϕ represent dependent constitutive quantities in general. Substituting the forms (30) for the energy fields into the local form $(29)_1$ for total energy balance yields the result

$$\dot{\varepsilon} + \operatorname{div} \boldsymbol{q} - r = \boldsymbol{P} \cdot \nabla\dot{\xi} - \boldsymbol{z} \cdot \dot{\xi} + \tfrac{1}{2}\, c\, \dot{\xi} \cdot \dot{\xi} \tag{31}$$

for this balance. Appearing here are the field

$$c := \dot{\varrho} \tag{32}$$

associated with mass balance, and that

$$\boldsymbol{z} := \dot{\boldsymbol{m}} - \operatorname{div} \boldsymbol{P} - \boldsymbol{f} \tag{33}$$

associated with momentum balance, where

$$\boldsymbol{m} := \varrho \dot{\xi}$$

represents the usual continuum momentum density. As discussed by, e.g., Šilhavý (1997, Ch. 6), in the context of the usual transformation relations for the fields appearing in (31) under change of Euclidean observer, one can show that necessary conditions for the Euclidean frame-indifference of $(29)_1$ in the form (31) are the mass

$$c = 0 \quad \Longrightarrow \quad \dot{\varrho} = 0 \tag{34}$$

via (32), momentum

$$\boldsymbol{z} = \mathbf{0} \quad \Longrightarrow \quad \dot{\boldsymbol{m}} = \operatorname{div} \boldsymbol{P} + \boldsymbol{f} \tag{35}$$

via (33), and moment of momentum

$$\boldsymbol{S}^{\mathrm{T}} = \boldsymbol{S} \tag{36}$$

balances, respectively, the latter with respect to the second Piola-Kirchhoff stress $\boldsymbol{S} = \boldsymbol{F}^{-1}\boldsymbol{P}$. As such, beyond a constant (i.e., in time) mass density, we obtain the standard forms

$$\begin{aligned} \dot{\boldsymbol{m}} &= \mathbf{0} + \operatorname{div} \boldsymbol{P} + \boldsymbol{f} \,, \\ \dot{\varepsilon} &= \tfrac{1}{2}\boldsymbol{S} \cdot \dot{\boldsymbol{C}} - \operatorname{div} \boldsymbol{q} + r \,, \end{aligned} \tag{37}$$

for local balance of continuum momentum and internal energy, respectively, in the current context via (31), (35) and (36).

We turn next to thermodynamic considerations. As shown in effect by Maugin (1990), one approach to the formulation of the entropy principle for material behaviour depending on internal variables and their gradients can be based upon a weaker form of the dissipation (rate) inequality than the usual Clausius-Duhem relation. This form follows from the local entropy (29) and internal energy $(37)_2$ balances via the Clausius-Duhem form

$$\sigma = r/\theta \tag{38}$$

for the entropy supply rate σ density in terms of the internal energy supply rate density r and temperature θ. Indeed, this leads to the expression

$$\delta = \tfrac{1}{2}\boldsymbol{S} \cdot \dot{\boldsymbol{C}} - \dot{\psi} - \eta\,\dot{\theta} + \operatorname{div}(\theta\boldsymbol{\phi} - \boldsymbol{q}) - \boldsymbol{\phi} \cdot \nabla\theta \tag{39}$$

for the dissipation rate density

$$\delta := \theta\pi \tag{40}$$

via $(37)_2$, where

$$\psi := \varepsilon - \theta\,\eta \tag{41}$$

represents the referential free energy density. Substituting next the form (28) for ψ into (39) yields that

$$\begin{aligned} \delta &= \{\tfrac{1}{2}\boldsymbol{S} - \psi_{,\boldsymbol{C}}\} \cdot \dot{\boldsymbol{C}} - \{\eta + \psi_{,\theta}\}\,\dot{\theta} - \psi_{,\nabla} \cdot \nabla\dot{\theta} - \psi_{,\dot{\gamma}} \cdot \ddot{\gamma} - \psi_{,\nabla\dot{\gamma}} \cdot \nabla\ddot{\gamma} \\ &+ \operatorname{div}(\theta\boldsymbol{\phi} - \boldsymbol{q} - \Phi_{\mathrm{V}}^{\mathrm{T}}\dot{\gamma}) + (\varpi_{\mathrm{V}} + \operatorname{div}\Phi_{\mathrm{V}}) \cdot \dot{\gamma} - \boldsymbol{\phi} \cdot \nabla\theta \end{aligned} \tag{42}$$

for δ via (27). Here,

$$\varpi_{\mathrm{V}} := -\,K^{\mathrm{T}}\psi_{,\alpha} \quad , \tag{43}$$

$\varpi_{\rm V} := (\varpi_{\rm V1}, \ldots, \varpi_{{\rm V}m})$, and

$$\Phi_{\rm V} := \mathcal{J}^{\rm T}\psi_{,\,\alpha} \quad , \tag{44}$$

with $\Phi_{\rm V} := (\varphi_{\rm V1}, \ldots, \varphi_{{\rm V}m})$. Now, on the basis of (27) and (28), δ in (42) is linear in the fields $\dot{\boldsymbol{C}}$, $\dot{\theta}$, $\nabla\dot{\theta}$, $\ddot{\gamma}$ and $\nabla\ddot{\gamma}$. Consequently, the Coleman-Noll approach to the exploitation of the entropy inequality implies that $\delta \geq 0$ is insured for all thermodynamically-admissible processes iff the corresponding coefficients of these fields in (42) vanish, yielding the restrictions

$$\begin{aligned} \boldsymbol{S} &= 2\,\psi_{,\boldsymbol{C}}\ , \\ \eta &= -\psi_{,\,\theta}\ , \\ \boldsymbol{0} &= \psi_{,\,\nabla\theta}\ , \\ 0 &= \psi_{,\,\dot{\gamma}_{\mathfrak{a}}}\ , \quad \mathfrak{a} = 1, \ldots, m\ , \\ \boldsymbol{0} &= \psi_{,\,\nabla\dot{\gamma}_{\mathfrak{a}}}\ , \quad \mathfrak{a} = 1, \ldots, m\ , \end{aligned} \tag{45}$$

on the form of the referential free energy density ψ, as well as the reduced expression

$$\delta = \operatorname{div}(\theta\phi - \boldsymbol{q} - \Phi_{\rm V}^{\rm T}\dot{\gamma}) + (\varpi_{\rm V} + \operatorname{div}\Phi_{\rm V})\cdot\dot{\gamma} - \theta\phi\cdot\nabla\ln\theta \tag{46}$$

for δ as given by (42), representing its so-called residual form for the current constitutive class. In this case, then, the reduced form

$$\psi = \psi(\theta, \boldsymbol{C}, \alpha) \tag{47}$$

of ψ follows from (28) and (45).

On the basis of the residual form (46) for δ, assume next that, as dependent constitutive quantities, $\varpi_{\rm V} + \operatorname{div}\Phi_{\rm V}$ and ϕ are defined on convex subsets of the non-equilibrium part of the state space, representing the set of all admissible $\nabla\theta$, $\dot{\gamma}$ and $\nabla\dot{\gamma}$. If $\varpi_{\rm V} + \operatorname{div}\Phi_{\rm V}$ and ϕ, again as dependent constitutive quantities, are in addition continuously differentiable in $\nabla\theta$, $\dot{\gamma}$ and $\nabla\dot{\gamma}$ on the subset in question, one may generalize the results of Edelen (1973, 1985) to show[¶] that the requirement $\delta \geq 0$ on δ given by (46) yields the constitutive results

$$\begin{aligned} \varpi_{\rm V} + \operatorname{div}\Phi_{\rm V} &= d_{{\rm V},\,\dot{\gamma}} - \operatorname{div} d_{{\rm V},\,\nabla\dot{\gamma}} + \zeta_{{\rm V}\,\dot{\gamma}}\ , \\ -\theta\phi &= d_{{\rm V},\,\nabla\ln} + \zeta_{{\rm V}\,\nabla\ln}\ , \end{aligned} \tag{48}$$

for $\varpi_{\rm V} + \operatorname{div}\Phi_{\rm V}$ and ϕ, respectively, in terms of the dissipation potential

$$d_{\rm V} = d_{\rm V}(\theta, \boldsymbol{C}, \alpha, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma}) \tag{49}$$

and constitutive quantities

$$\begin{aligned} \zeta_{{\rm V}\,\dot{\gamma}} &= \zeta_{{\rm V}\,\dot{\gamma}}(\theta, \boldsymbol{C}, \alpha, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma})\ , \\ \zeta_{{\rm V}\,\nabla\ln} &= \zeta_{{\rm V}\,\nabla\ln}(\theta, \boldsymbol{C}, \alpha, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma})\ , \end{aligned}$$

which satisfy

$$\zeta_{{\rm V}\,\dot{\gamma}}\cdot\dot{\gamma} + \zeta_{{\rm V}\,\nabla\ln}\cdot\nabla\ln\theta = 0 \quad , \tag{50}$$

[¶]In fact, this can be shown for the weaker case of simply-connected, rather than convex, subsets of the dynamic part of state space via homotopy (see, e.g., Abraham et al. 1988, proof of Lemma 6.4.14).

i.e., they do not contribute to δ. To simplify the rest of the formulation, it is useful to work with the stronger constitutive assumption that d_{V} exists, in which case $\zeta_{\mathrm{V}\,\dot{\gamma}}$ and $\zeta_{\mathrm{V}\,\nabla\ln}$ vanish identically. On the basis then of the *constitutive form*

$$\phi \mathrel{\widehat{=}} \theta^{-1}\boldsymbol{q} + \theta^{-1}(\Phi_{\mathrm{V}} + d_{\mathrm{V},\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} \tag{51}$$

for the entropy flux density, δ is determined by the form of d_{V} alone, i.e.,

$$\delta = d_{\mathrm{V},\,\dot{\gamma}} \cdot \dot{\gamma} + d_{\mathrm{V},\,\nabla\dot{\gamma}} \cdot \nabla\dot{\gamma} + d_{\mathrm{V},\,\nabla\ln} \cdot \nabla\ln\theta \quad . \tag{52}$$

Among other things, (52) implies that a convex dependence of d_{V} on the non-equilibrium fields is sufficient, but not necessary, to satisfy $\delta \geq 0$. Indeed, with $d_{\mathrm{V}}(\theta, \boldsymbol{C}, \alpha, \mathbf{0}, \mathbf{0}, \mathbf{0}) = 0$, d_{V} is convex in $\nabla\theta$, $\dot{\gamma}$ and $\nabla\dot{\gamma}$ if $\delta \geq d_{\mathrm{V}}$ (i.e., with δ given by (52)) for given values of the other variables. So, if d_{V} is convex in $\nabla\theta$ and $\dot{\gamma}$, and $d_{\mathrm{V}} \geq 0$, then $\delta \geq 0$ is satisfied. On the other hand, even if $d_{\mathrm{V}} \geq 0$, $\delta \geq 0$ does not necessarily require $\delta \geq d_{\mathrm{V}}$, i.e., d_{V} convex.

Lastly, in the context of the entropy balance $(29)_2$, the constitutive assumption (38), together with (40) and the results $(45)_{1,2}$, (46) and (48), lead to the expression

$$c\,\dot{\theta} = \tfrac{1}{2}\,\theta\boldsymbol{S}_{,\,\theta} \cdot \dot{\boldsymbol{C}} + \omega_{\mathrm{V}} + \operatorname{div} d_{\mathrm{V},\,\nabla\ln} + r \tag{53}$$

for the evolution of θ via (47) and (49). Here,

$$c := -\,\theta\psi_{,\,\theta\theta} \tag{54}$$

represents the heat capacity at constant γ, $\boldsymbol{C}$, and so on, $\frac{1}{2}\,\theta\boldsymbol{S}_{,\,\theta} \cdot \dot{\boldsymbol{C}} = \theta\psi_{,\,\theta\boldsymbol{C}} \cdot \dot{\boldsymbol{C}}$ the rate (density) of heating due to thermoelastic processes, and

$$\omega_{\mathrm{V}} := (d_{\mathrm{V},\,\dot{\gamma}} + \theta\,\mathcal{K}^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \dot{\gamma} + (d_{\mathrm{V},\,\nabla\dot{\gamma}} + \theta\,\mathcal{J}^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \nabla\dot{\gamma} \tag{55}$$

that due to inelastic processes via (27). In addition, $(48)_1$ implies the result

$$d_{\mathrm{V},\,\dot{\gamma}} = \operatorname{div}(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} + d_{\mathrm{V},\,\nabla\dot{\gamma}}) - \mathcal{K}^{\mathrm{T}}\psi_{,\,\alpha} \tag{56}$$

for the evolution of γ via (43) and (44). Finally,

$$-\boldsymbol{q} = d_{\mathrm{V},\,\nabla\ln} + (\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} + d_{\mathrm{V},\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} \tag{57}$$

follows for the heat flux density $\boldsymbol{q}$ from (51) and $(48)_2$. As such, the dependence of ψ on α, as well as that of d_{V} on $\nabla\dot{\gamma}$, lead in general to additional contributions to $\boldsymbol{q}$ in the context of the modeling of the γ as GIVs.

This completes the formulation of balance relations and the thermodynamic analysis for the modeling of the γ as GIVs. Next, we carry out such a formulation for the case that the γ are modeled as internal DOFs.

5. Internal degrees-of-freedom model for glide-system slips

Alternative to the model for the glide-system slips as GIVs in the sense of the last section is that in which they are interpreted as so-called internal degrees-of-freedom (DOFs). In this case, the degrees-of-freedom[‖] of the material consist of (i), the usual "external" continuum DOFs

[‖]This entails a generalization of the classical concept of "degree-of-freedom" to materials with structure.

represented by the motion ξ, and (ii), the "internal" DOFs γ. Or to use the terminology of Capriz (1989), the γ are modeled here as scalar-valued continuum microstructural fields. Once established as DOFs, the modeling of the γ proceeds by formal analogy with that of ξ, the only difference being that, in contrast to external DOFs represented by ξ, each internal DOF $\gamma_{\mathfrak{a}}$ is (i.e., by assumption) Euclidean frame-indifferent. Otherwise, the analogy is complete. In particular, each $\gamma_{\mathfrak{a}}$ is assumed to contribute to the total energy, the total energy flux and total energy supply, of the material in a fashion formally analogous to ξ, i.e.,

$$\begin{array}{lcccccc} e & = & \varepsilon & + & \frac{1}{2}\,\dot{\xi}\cdot\varrho\dot{\xi} & + & \frac{1}{2}\,\dot{\gamma}\cdot\varrho\mathbf{I}\dot{\gamma}\,, \\ \boldsymbol{h} & = & -\boldsymbol{q} & + & \boldsymbol{P}^{\mathrm{T}}\dot{\xi} & + & \Phi_{\mathrm{F}}^{\mathrm{T}}\dot{\gamma}\,, \\ s & = & r & + & \boldsymbol{f}\cdot\dot{\xi} & + & \varsigma\cdot\dot{\gamma}\,, \end{array} \tag{58}$$

for total energy density e, total energy flux density $\boldsymbol{h}$, and total energy supply rate density s. Here,

$$\mathbf{I} := \begin{bmatrix} \iota_{11} & \cdots & \iota_{1m} \\ \vdots & \ddots & \vdots \\ \iota_{m1} & \cdots & \iota_{mm} \end{bmatrix}$$

is the (symmetric, positive-definite) matrix of microinertia coefficients, $\Phi_{\mathrm{F}} := (\varphi_{\mathrm{F}1},\dots,\varphi_{\mathrm{F}m})$ the array of flux densities, and $\varsigma := (\varsigma_1,\dots,\varsigma_m)$ the array of external supply rate densities, associated with γ. For simplicity, we assume that $\mathbf{I}$ is constant in this work. Next, substitution of (58) into the general local form $(29)_1$ of total energy balance yields

$$\dot{\varepsilon} + \operatorname{div}\boldsymbol{q} - r = \boldsymbol{P}\cdot\nabla\dot{\xi} + \Phi_{\mathrm{F}}\cdot\nabla\dot{\gamma} - \boldsymbol{z}\cdot\dot{\xi} - \varpi_{\mathrm{F}}\cdot\dot{\gamma} + \tfrac{1}{2}\,c\,(\dot{\xi}\cdot\dot{\xi} + \dot{\gamma}\cdot\mathbf{I}\dot{\gamma}) \tag{59}$$

via (32) and (33). Here,

$$\varpi_{\mathrm{F}} := \dot{\mu} - \operatorname{div}\Phi_{\mathrm{F}} - \varsigma \tag{60}$$

is associated with the evolution of γ,

$$\mu := \varrho\,\mathbf{I}\,\dot{\gamma} \tag{61}$$

being the corresponding momentum density. Consider now the usual transformation relations for the field appearing in (58) and (59) under change of Euclidean observer, and in particular the assumed Euclidean frame-indifference of the elements of γ, $\mathbf{I}$, and Φ_{F}. As discussed in the last section, using these, one can show that necessary conditions for the Euclidean frame-indifference of $(29)_1$ in the form (59) are the mass (34), momentum (35), and moment of momentum (36) balances, respectively. As such, beyond a constant (i.e., in time) mass density, we obtain the set

$$\begin{array}{lccccccc} \dot{\boldsymbol{m}} & = & \mathbf{0} & + & \operatorname{div}\boldsymbol{P} & + & \boldsymbol{f}\,, \\ \dot{\mu} & = & \varpi_{\mathrm{F}} & + & \operatorname{div}\Phi_{\mathrm{F}} & + & \varsigma\,, \\ \dot{\varepsilon} & = & \frac{1}{2}\,\boldsymbol{S}\cdot\dot{\boldsymbol{C}} + \Phi_{\mathrm{F}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{F}}\cdot\dot{\gamma} & - & \operatorname{div}\boldsymbol{q} & + & r\,, \end{array} \tag{62}$$

of field relations via (35), (36), (59) and (60).

Since we are modeling the γ as (internal) DOFs in the current section, the relevant thermodynamic analysis is based on the usual Clausius-Duhem constitutive forms

$$\begin{array}{lcl} \phi & = & \boldsymbol{q}/\theta\,, \\ \sigma & = & r/\theta\,, \end{array} \tag{63}$$

for the entropy flux ϕ and supply rate σ densities, respectively. Substituting these into the entropy balance $(29)_2$, we obtain the result

$$\delta = \tfrac{1}{2}\,\boldsymbol{S}\cdot\dot{\boldsymbol{C}} + \Phi_{\mathrm{F}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{F}}\cdot\dot{\gamma} - \dot{\psi} - \eta\,\dot{\theta} - \theta^{-1}\boldsymbol{q}\cdot\nabla\theta \tag{64}$$

for the dissipation rate density $\delta := \theta\pi$ via $(62)_3$ via (41). In turn, substitution of the constitutive form (28) for the free energy ψ into (64), and use of that (27) for α, yields

$$\begin{aligned}\delta &= \{\tfrac{1}{2}\,\boldsymbol{S} - \psi_{,\boldsymbol{C}}\}\cdot\dot{\boldsymbol{C}} - \{\eta + \psi_{,\theta}\}\,\dot{\theta} - \psi_{,\nabla\theta}\cdot\nabla\dot{\theta} - \theta^{-1}\boldsymbol{q}\cdot\nabla\theta \\ &+ \Phi_{\mathrm{FN}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{FN}}\cdot\dot{\gamma} - \psi_{,\dot{\gamma}}\cdot\ddot{\gamma} - \psi_{,\nabla\dot{\gamma}}\cdot\nabla\ddot{\gamma}\ ,\end{aligned} \tag{65}$$

with

$$\begin{aligned}\Phi_{\mathrm{FN}} &:= \Phi_{\mathrm{F}} - \mathcal{J}^{\mathrm{T}}\psi_{,\alpha}\ ,\\ \varpi_{\mathrm{FN}} &:= \varpi_{\mathrm{F}} + K^{\mathrm{T}}\psi_{,\alpha}\ ,\end{aligned} \tag{66}$$

the non-equilibrium parts of Φ_{F} and ϖ_{F}, respectively. On the basis of (28), δ is linear in the independent fields $\dot{\boldsymbol{C}}$, $\dot{\theta}$, $\nabla\dot{\theta}$, $\ddot{\gamma}$ and $\nabla\ddot{\gamma}$. As such, in the context of the Coleman-Noll approach to the exploitation of the entropy inequality, $\delta \geq 0$ is insured for all thermodynamically-admissible processes iff the corresponding coefficients of these fields in (65) vanish, yielding

$$\begin{aligned}\boldsymbol{S} &= 2\,\psi_{,\boldsymbol{C}}\ ,\\ \eta &= -\psi_{,\theta}\ ,\\ \boldsymbol{0} &= \psi_{,\nabla\theta}\ ,\\ 0 &= \psi_{,\dot{\gamma}_{\mathfrak{a}}}\ , \quad \mathfrak{a} = 1,\ldots,m\ ,\\ \boldsymbol{0} &= \psi_{,\nabla\dot{\gamma}_{\mathfrak{a}}}\ , \quad \mathfrak{a} = 1,\ldots,m\ .\end{aligned} \tag{67}$$

As in the last section, these restrictions also result in the reduced form (47) for ψ. Consequently, the constitutive fields $\boldsymbol{S}$, ε and η are determined in terms of ψ as given by (47). On the other hand, the Φ_{FN}, ϖ_{FN} as well as $\boldsymbol{q}$ still take the general form (28). These are restricted further in the context of the residual form

$$\delta = \Phi_{\mathrm{FN}}\cdot\nabla\dot{\gamma} - \varpi_{\mathrm{FN}}\cdot\dot{\gamma} - \theta^{-1}\boldsymbol{q}\cdot\nabla\theta$$

for δ in the current constitutive class from (67). Treating Φ_{FN}, ϖ_{FN} and $\boldsymbol{q}$ constitutively in a fashion analogous to $\varpi_{\mathrm{V}} + \operatorname{div}\Phi_{\mathrm{V}}$ and ϕ from the last section in the context of (48), the requirement $\delta \geq 0$ results in the constitutive forms

$$\begin{aligned}\Phi_{\mathrm{FN}} &= d_{\mathrm{F},\nabla\dot{\gamma}} + \zeta_{\mathrm{F}\,\nabla\dot{\gamma}}\ ,\\ -\varpi_{\mathrm{FN}} &= d_{\mathrm{F},\dot{\gamma}} + \zeta_{\mathrm{F}\,\dot{\gamma}}\ ,\\ -\boldsymbol{q} &= d_{\mathrm{F},\nabla\ln} + \zeta_{\mathrm{F}\,\nabla\ln}\ ,\end{aligned} \tag{68}$$

for these in terms of a dissipation potential d_{F} and corresponding constitutive quantities $\zeta_{\mathrm{F}\,\nabla\dot{\gamma}}$, $\zeta_{\mathrm{F}\,\dot{\gamma}}$ and $\zeta_{\mathrm{F}\,\nabla\ln}$, all of the general reduced material-frame-indifferent form (28). As in the last section, the latter three are dissipationless, i.e.,

$$\zeta_{\mathrm{F}\,\dot{\gamma}}\cdot\dot{\gamma} + \zeta_{\mathrm{F}\,\nabla\dot{\gamma}}\cdot\nabla\dot{\gamma} + \zeta_{\mathrm{F}\,\nabla\ln}\cdot\nabla\ln\theta = 0 \tag{69}$$

analogous to (50) in the GIV case. Consequently, δ reduces to

$$\delta = d_{\mathrm{F},\,\dot{\gamma}} \cdot \dot{\gamma} + d_{\mathrm{F},\,\nabla\dot{\gamma}} \cdot \nabla\dot{\gamma} + d_{\mathrm{F},\,\nabla\ln} \cdot \nabla\ln\theta$$

via (68) and (69), analogous to (52) in the GIV case. In what follows, we again, as in the last section, work for simplicity with the stronger constitutive assumption that d_{F} exists, in which case $\zeta_{\mathrm{F}\,\dot{\gamma}}$, $\zeta_{\mathrm{F}\,\nabla\dot{\gamma}}$ and $\zeta_{\mathrm{F}\,\nabla\ln}$ vanish identically.

On the basis of the above assumptions and results, then, the field relation

$$c\,\dot{\theta} = \tfrac{1}{2}\,\theta\,\boldsymbol{S}_{,\,\theta} \cdot \dot{\boldsymbol{C}} + \omega_{\mathrm{F}} + \operatorname{div} d_{\mathrm{F},\,\nabla\ln} + r \tag{70}$$

for temperature evolution analogous to (53) is obtained in the current context via (54), with

$$\omega_{\mathrm{F}} := (d_{\mathrm{F},\,\dot{\gamma}} + \theta\,K^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \dot{\gamma} + (d_{\mathrm{F},\,\nabla\dot{\gamma}} + \theta\,\mathcal{J}^{\mathrm{T}}\psi_{,\,\theta\alpha}) \cdot \nabla\dot{\gamma} \tag{71}$$

the rate of heating due to inelastic processes analogous to ω_{V} from (55). Finally, $(68)_{1,2}$ lead to the form

$$\varrho\mathbf{I}\ddot{\gamma} + d_{\mathrm{F},\,\dot{\gamma}} = \operatorname{div}(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha} + d_{\mathrm{F},\,\nabla\dot{\gamma}}) - K^{\mathrm{T}}\psi_{,\,\alpha} + \varsigma \tag{72}$$

for the evolution of γ via (61), $(62)_2$ and (66).

With the general thermodynamic framework established in the last two sections now in hand, the next step is the formulation of specific models for GND development and their incoporation into this framework, our next task.

6. Effective models for GNDs

The first model for GNDs to be considered in this section is formulated at the glide-system level. As it turns out, this model represents a three-dimensional generalization of the model of Ashby (1970), who showed that the development of GNDs in a given glide system is directly related to the inhomogeneity of inelastic deformation in this system. In particular, in the current finite-deformation context, this generalization is based on the incompatibility of $\boldsymbol{F}_{\mathfrak{a}}$ with respect to the reference placement. To this end, consider the vector measure**

$$\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C) := \oint_C \boldsymbol{F}_{\mathfrak{a}}\,\boldsymbol{t}_C = \oint_C \gamma_{\mathfrak{a}}\,(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{t}_C)\,\boldsymbol{s}_{\mathfrak{a}} \tag{73}$$

of the length of glide-system GNDs around an *arbitrary* closed curve or circuit C in the reference configuration, the second form following from (20). Here, $\boldsymbol{t}_C$ represents the unit tangent to C oriented *clockwise*. Alternatively, $\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C)$ is given by††

$$\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C) := \oint_C \boldsymbol{F}_{\mathfrak{a}}\,\boldsymbol{t}_C = \int_S (\operatorname{curl}\boldsymbol{F}_{\mathfrak{a}})\boldsymbol{n}_S \tag{74}$$

with respect to the material surface S bounded by C via Stokes theorem. Here,

$$\operatorname{curl}\boldsymbol{F}_{\mathfrak{a}} = (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})(\boldsymbol{I} \times \nabla\gamma_{\mathfrak{a}}) = \boldsymbol{s}_{\mathfrak{a}} \otimes (\nabla\gamma_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}}) \tag{75}$$

**Volume dv, surface da and line $d\ell$ elements are suppressed in the corresponding integrals appearing in what follows for notational simplicity. Unless otherwise stated, all such integrals to follow are with respect to line, surfaces and/or parts of the arbitrary global reference placement of the material body under consideration.

††Note that curl $\boldsymbol{F}_{\mathfrak{a}}$ appearing in (74) is consistent with the form (8) for the curl of a second-order Euclidean tensor field.

from (7), (20), and the constancy of $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$. On the basis of (74), $\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C)$ can also be interpreted as a vector measure of the total length of GNDs piercing the material surface S enclosed by C. The quantity curl $\boldsymbol{F}_\mathfrak{a}$ determines in particular the dislocation density tensor $\alpha^{(I)}$ worked with recently by Shizawa and Zbib (1999) as based on the incompatibility of their slip tensor $\gamma^{(I)} := \sum_{\mathfrak{a}=1}^{n} \gamma_\mathfrak{a}\, \boldsymbol{s}_\mathfrak{a} \otimes \boldsymbol{n}_\mathfrak{a}$. Indeed, we have $\alpha^{(I)} := \operatorname{curl} \gamma^{(I)} = \sum_{\mathfrak{a}=1}^{n} \operatorname{curl} \boldsymbol{F}_\mathfrak{a}$ in the current notation.

Now, from (73) and the constancy of $\boldsymbol{s}_\mathfrak{a}$, note that $\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C)$ is parallel to the slip direction $\boldsymbol{s}_\mathfrak{a}$, i.e.,

$$\boldsymbol{l}_{\mathrm{G}\mathfrak{a}}(C) = l_{\mathrm{G}\mathfrak{a}}\, \boldsymbol{s}_\mathfrak{a}$$

with

$$l_{\mathrm{G}\mathfrak{a}}(C) := \oint_C \gamma_\mathfrak{a}\, \boldsymbol{n}_\mathfrak{a} \cdot \boldsymbol{t}_C = \int_S (\operatorname{curl} \boldsymbol{F}_\mathfrak{a})^{\mathrm{T}} \boldsymbol{s}_\mathfrak{a} \cdot \boldsymbol{n}_S \tag{76}$$

the scalar length of GNDs piercing S via (74). With the help of a characteristic Burgers vector magnitude b, this length can be written in the alternative form

$$l_{\mathrm{G}\mathfrak{a}}(C) = b \int_S \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} \cdot \boldsymbol{n}_S \tag{77}$$

in terms of the vector field $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ determined by

$$\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} := b^{-1} (\operatorname{curl} \boldsymbol{F}_\mathfrak{a})^{\mathrm{T}} \boldsymbol{s}_\mathfrak{a} = b^{-1}\, \nabla\gamma_\mathfrak{a} \times \boldsymbol{n}_\mathfrak{a} \quad . \tag{78}$$

From the dimensional point of view, $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ represents a (vector-valued) GND surface (number) density. As such, the projection $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} \cdot \boldsymbol{n}_S$ of $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ onto S gives the (scalar) surface (number) density of such GNDs piercing S. The projection of (78) onto the glide-system basis $(\boldsymbol{s}_\mathfrak{a}, \boldsymbol{n}_\mathfrak{a}, \boldsymbol{t}_\mathfrak{a})$ yields

$$\begin{aligned} \boldsymbol{s}_\mathfrak{a} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} &= -b^{-1}\, \boldsymbol{t}_\mathfrak{a} \cdot \nabla\gamma_\mathfrak{a} \,, \\ \boldsymbol{t}_\mathfrak{a} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{s}_\mathfrak{a} \cdot \nabla\gamma_\mathfrak{a} \,, \\ \boldsymbol{n}_\mathfrak{a} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} &= 0 \,, \end{aligned} \tag{79}$$

for the case of constant b. In particular, the first two of these expressions are consistent with two-dimensional results of Ashby (1970) for the GND density with respect to the slip direction and that perpendicular to it in the glide plane generalized to three dimensions. Such three-dimensional relations are also obtained in the recent crystallographic approach to GND modeling of Arsenlis and Parks (1999). Likewise in agreement with the model of Ashby (1970) is the fact that $(79)_3$ implies that there is no GND development perpendicular to the glide plane (i.e., parallel to $\boldsymbol{n}_\mathfrak{a}$) in this model. ¿From another point of view, if $\nabla\gamma_\mathfrak{a}$ were parallel to $\boldsymbol{n}_\mathfrak{a}$, there would be no GND development at all in this model; indeed, as shown by (75), in this case, $\boldsymbol{F}_\mathfrak{a}$ would be compatible.

The second class of GND models considered in this work is based on the vector measure

$$\boldsymbol{l}_{\mathrm{G}}(C) := \oint_C \boldsymbol{F}_{\mathrm{P}}\, \boldsymbol{t}_C \;=\; \int_S (\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}) \boldsymbol{n}_S \tag{80}$$

of the length of GNDs from all glide systems around C in the material as measured by the incompatibility of the local inelastic deformation $\boldsymbol{F}_{\mathrm{P}}$. In particular, the phenomenological GND model of Dai and Parks (1997), utilized by them to model grain-size effects in polycrystalline metals, applied as well recently by Busso et al. (2000) to model size effects in nickel-based superalloys, is of this type. In a different context, the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ has also been used recently by Ortiz and Repetto (1999), as well as by Ortiz et al. (2000), to model in an effective fashion the contribution of the dislocation self- or core energy to the total free energy of ductile single crystals. In what follows, we refer to the GND model based on the measure (80) as the continuum (GND) model. To enable comparison of this continuum GND model with the glide-system model discussed above, it is useful to express the former in terms of glide-system quantities formally analogous to those appearing in the latter. To this end, note that the evolution relation (24) for $\boldsymbol{F}_{\mathrm{P}}$ induces the glide-system decomposition

$$\boldsymbol{l}_{\mathrm{G}}(C) = \sum\nolimits_{\mathfrak{a}=1}^{n} l_{\mathrm{G}\mathfrak{a}}(C)\, \boldsymbol{s}_{\mathfrak{a}}$$

of $\boldsymbol{l}_{\mathrm{G}}(C)$ in terms of the set $l_{\mathrm{G}1}(C), \ldots, l_{\mathrm{G}n}(C)$ of glide-system GND lengths with respect to C formally analogous to those (76) in the context of the glide-system GND model. In contrast to this latter case, however, each $l_{\mathrm{G}\mathfrak{a}}$ here is determined by an evolution relation, i.e.,

$$\dot{l}_{\mathrm{G}\mathfrak{a}}(C) = \oint_C \dot{\gamma}_{\mathfrak{a}}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{t}_C = \int_S \operatorname{curl}(\dot{\boldsymbol{F}}_{\mathfrak{a}} \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{n}_S \quad , \tag{81}$$

with

$$\operatorname{curl}(\dot{\boldsymbol{F}}_{\mathfrak{a}} \boldsymbol{F}_{\mathrm{P}}) = (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}})(\boldsymbol{I} \times \nabla \dot{\gamma}_{\mathfrak{a}}) + \boldsymbol{s}_{\mathfrak{a}} \otimes (\operatorname{curl} \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}\, \dot{\gamma}_{\mathfrak{a}}$$

via (7) and (20). Alternatively, we can express $l_{\mathrm{G}\mathfrak{a}}(C)$ as determined by (81) in the form (77) involving the vector-valued GND surface density $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$, with now

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = b^{-1} \operatorname{curl}(\dot{\boldsymbol{F}}_{\mathfrak{a}} \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{s}_{\mathfrak{a}} = b^{-1}\, \nabla \dot{\gamma}_{\mathfrak{a}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} + b^{-1} (\operatorname{curl} \boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}\, \dot{\gamma}_{\mathfrak{a}} \tag{82}$$

in the context of (80). As implied by the notation, $\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}}$ from (82) in the current context is formally analogous to the time-derivative of (78) in the glide-system GND model. Now, from the results (26) and (82), we have

$$\dot{\overline{\operatorname{curl} \boldsymbol{F}_{\mathrm{P}}}} = b \sum\nolimits_{\mathfrak{a}=1}^{m} \boldsymbol{s}_{\mathfrak{a}} \otimes \dot{\boldsymbol{g}}_{\mathfrak{a}}$$

and so the expression[‡‡]

$$\operatorname{curl} \boldsymbol{F}_{\mathrm{P}} = b \sum\nolimits_{\mathfrak{a}=1}^{n} \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{g}_{\mathfrak{a}}$$

for the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ in terms of the set $(\boldsymbol{g}_1, \ldots, \boldsymbol{g}_n)$ of vector-valued GND densities. Substituting this result into (82) then yields

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \sum\nolimits_{\mathfrak{b} \neq \mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} + b^{-1}\, \nabla \dot{\gamma}_{\mathfrak{a}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}}$$

with $\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{a}} = 0$ and $\sum_{\mathfrak{b} \neq \mathfrak{a}} := \sum_{\mathfrak{b}=1, \mathfrak{b} \neq \mathfrak{a}}^{m}$. Relative to $(\boldsymbol{s}_{\mathfrak{a}}, \boldsymbol{n}_{\mathfrak{a}}, \boldsymbol{t}_{\mathfrak{a}})$, note that

$$\begin{aligned}
\boldsymbol{s}_{\mathfrak{a}} \cdot \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{s}_{\mathfrak{a}} \cdot \nabla \dot{\gamma}_{\mathfrak{a}} &+& \sum\nolimits_{\mathfrak{b} \neq \mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} \,, \\
\boldsymbol{t}_{\mathfrak{a}} \cdot \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{t}_{\mathfrak{a}} \cdot \nabla \dot{\gamma}_{\mathfrak{a}} &+& \sum\nolimits_{\mathfrak{b} \neq \mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{t}_{\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} \,, \\
\boldsymbol{n}_{\mathfrak{a}} \cdot \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= b^{-1}\, \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} \boldsymbol{n}_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}} \cdot \nabla \dot{\gamma}_{\mathfrak{a}} &+& \sum\nolimits_{\mathfrak{b} \neq \mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} \,,
\end{aligned}$$

via (8) and (21), analogous to (79). In contrast to the glide-system GND model, then, this approach does lead to a development of (edge) GNDs perpendicular to the glide plane (i.e., parallel to $\boldsymbol{n}_{\mathfrak{a}}$).

[‡‡]Assuming the integration constant to be zero for simplicity, i.e., that there is no initial inelastic incompatibility.

To summarize then, we have the expressions

$$
\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \begin{cases} b^{-1}\,\overline{\nabla\gamma_{\mathfrak{a}}}^{\boldsymbol{\cdot}} \times \boldsymbol{n}_{\mathfrak{a}} & \text{glide-system model} \\ b^{-1}\,\overline{\nabla\gamma_{\mathfrak{a}}}^{\boldsymbol{\cdot}} \times \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} + \sum_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}}\cdot\boldsymbol{s}_{\mathfrak{b}})\,\boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\,\dot{\gamma}_{\mathfrak{a}} & \text{continuum model} \end{cases} \tag{83}
$$

for the evolution of the vector-valued measure $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ of GND density from the glide-system and continuum models discussed above. With these in hand, we are now ready to extend existing models for crystal plasticity to account for the effects of GNDs on their material behaviour, and in particular their effect on the hardening behaviour of the material. In the current thermodynamic context, such extensions are realized via the constitutive dependence of the free energy on GND density, and more generally on the dislocation state in the material, our next task.

7. Free energy and GNDs

With GND models such as those from the last section in hand, the question arises as to how these can be incoporated into the thermodynamic formulation for crystal plasticity developed in the previous sections. Since this formulation is determined predominantly by the free energy density ψ and dissipation potential d, this question becomes one of (i), which quantities characterize effectively (i.e., phenomenologically) the GND, and more generally dislocation, state of each material point $p \in B$, and (ii), how do ψ and d depend on these? The purpose of this section is to explore these issues for the case of the referential free energy density ψ. In particular, this involves the choice for α.

Among the possible measures of the inelastic/dislocation state of each material point, we have the arrays $\rho_{\mathrm{S}} = (\rho_{\mathrm{S}1},\ldots,\rho_{\mathrm{S}n})$ and $g_{\mathrm{G}} = (\boldsymbol{g}_{\mathrm{G}1},\ldots,\boldsymbol{g}_{\mathrm{G}n})$ of glide-system effective SSD and GND densities, respectively. Choosing then $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \rho_{\mathrm{S}}, g_{\mathrm{G}})$, ψ takes the form

$$
\psi(\theta,\boldsymbol{C},\alpha) = \psi_{\mathrm{D}}(\theta,\boldsymbol{C},\boldsymbol{F}_{\mathrm{P}},\rho_{\mathrm{S}},g_{\mathrm{G}})
$$

for ψ from (47), with

$$
\begin{aligned} \dot{\rho}_{\mathrm{S}\mathfrak{a}} &= \textstyle\sum_{\mathfrak{b}=1}^{m} K_{\mathrm{S}\mathfrak{a}\mathfrak{b}}\,\dot{\gamma}_{\mathfrak{b}}\,, \\ \dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} &= \textstyle\sum_{\mathfrak{b}=1}^{m} \boldsymbol{k}_{\mathrm{G}\mathfrak{a}\mathfrak{b}}\,\dot{\gamma}_{\mathfrak{b}} + \boldsymbol{J}_{\mathrm{G}\mathfrak{a}\mathfrak{b}}\nabla\dot{\gamma}_{\mathfrak{b}}\,, \end{aligned} \tag{84}
$$

from (27). This choice induces the decompositions

$$
\begin{aligned} \mathcal{K}^{\mathrm{T}}\psi_{,\alpha} &= (\dot{\boldsymbol{F}}_{\mathrm{P},\dot{\gamma}})^{\mathrm{T}}\psi_{\mathrm{D},\boldsymbol{F}_{\mathrm{P}}} &+\quad& \mathcal{K}_{\mathrm{S}}^{\mathrm{T}}\psi_{\mathrm{D},\rho_{\mathrm{S}}} &+\quad& \mathcal{K}_{\mathrm{G}}^{\mathrm{T}}\psi_{\mathrm{D},g_{\mathrm{G}}}\,, \\ \mathcal{J}^{\mathrm{T}}\psi_{,\alpha} &= 0 &+\quad& 0 &+\quad& \mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\psi_{\mathrm{D},g_{\mathrm{G}}}\,, \end{aligned} \tag{85}
$$

from (24) of the constitutive quantities $\mathcal{K}^{\mathrm{T}}\psi_{,\alpha}$ and $\mathcal{J}^{\mathrm{T}}\psi_{,\alpha}$ determining the form (56) or (72) of the field relation for γ. In particular, the models (83) for $\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}}$ yield

$$
\boldsymbol{k}_{\mathrm{G}\mathfrak{a}\mathfrak{b}} = \begin{cases} 0 & \text{glide-system model} \\ \delta_{\mathfrak{a}\mathfrak{b}} \sum_{\mathfrak{c}\neq\mathfrak{b}} (\boldsymbol{n}_{\mathfrak{b}}\cdot\boldsymbol{s}_{\mathfrak{c}})\,\boldsymbol{g}_{\mathrm{G}\mathfrak{c}} & \text{continuum model} \end{cases} \tag{86}
$$

and

$$
\boldsymbol{J}_{\mathrm{G}\mathfrak{a}\mathfrak{b}} = b^{-1}\,\delta_{\mathfrak{a}\mathfrak{b}} \begin{cases} \boldsymbol{I}\times\boldsymbol{n}_{\mathfrak{b}} & \text{glide-system model} \\ \boldsymbol{I}\times\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{b}} & \text{continuum model} \end{cases} \tag{87}
$$

for $\boldsymbol{k}_{\mathrm{G}\mathfrak{ab}}$ and $\boldsymbol{J}_{\mathrm{G}\mathfrak{ab}}$, respectively. And from (87), we have

$$(88)\qquad (\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha})_{\mathfrak{a}} = (\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{D},\,g_{\mathrm{G}}})_{\mathfrak{a}} = b^{-1}\begin{cases} \boldsymbol{n}_{\mathfrak{a}} \times \psi_{\mathrm{D},\,\boldsymbol{g}_{\mathfrak{a}}} & \text{glide-system model} \\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times \psi_{\mathrm{D},\,\boldsymbol{g}_{\mathfrak{a}}} & \text{continuum model} \end{cases}$$

for the flux contribution appearing in the evolution relation (56) or (72) for γ. From (84), $(85)_1$ and (86), we have

$$(K^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} = -\tau_{\mathfrak{a}} + x_{\mathfrak{a}} + \mathrm{sgn}(\dot{\gamma}_{\mathfrak{a}})\,r_{\mathfrak{a}}$$

where

$$(89)\qquad \tau_{\mathfrak{a}} = -((\dot{\boldsymbol{F}}_{\mathrm{P},\,\dot{\gamma}})^{\mathrm{T}}\psi_{,\,\boldsymbol{F}_{\mathrm{P}}})_{\mathfrak{a}} = -(\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})\boldsymbol{F}_{\mathrm{P}} \cdot \psi_{,\,\boldsymbol{F}_{\mathrm{P}}}$$

represents the glide-system Schmid stress via (24),

$$(90)\qquad x_{\mathfrak{a}} := \begin{cases} 0 & \text{glide-system model} \\ \sum_{\mathfrak{b}\neq\mathfrak{a}}(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,\psi_{\mathrm{D},\,\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}} & \text{continuum model} \end{cases}$$

(a contribution to) the glide-system back stress, and

$$(91)\qquad r_{\mathfrak{a}} := \sum_{\mathfrak{b}=1}^{m} I_{\mathrm{S}\mathfrak{ba}}\,\psi_{\mathrm{D},\,\rho_{\mathrm{S}\mathfrak{b}}}$$

the glide-system yield stress, with $K_{\mathrm{S}\mathfrak{ba}} = I_{\mathrm{S}\mathfrak{ba}}\,\mathrm{sgn}(\dot{\gamma}_{\mathfrak{b}})$. Note that $\mathrm{sgn}(\dot{\gamma}_{\mathfrak{a}})$ is a constitutive quantity in existing crystal plasticity models. For example, in the case of the (non-thermodynamic) glide-system flow rule

$$(92)\qquad \dot{\gamma}_{\mathfrak{a}} = \dot{\gamma}_{\mathfrak{a}\,0}\left|\frac{\tau_{\mathfrak{a}}}{\tau_{\mathrm{C}\mathfrak{a}}}\right|^{n}\mathrm{sgn}(\tau_{\mathfrak{a}})$$

of Teodosiu and Sideroff (1976) (similar to the form used by Asaro and Needleman, 1985; see also Teodosiu, 1997), we have $\mathrm{sgn}(\dot{\gamma}_{\mathfrak{a}}) \mathrel{\widehat{=}} \mathrm{sgn}(\tau_{\mathfrak{a}})$. Here, $\tau_{\mathrm{C}\mathfrak{a}}$ represents the critical Schmid stress for slip. In particular, such a constitutive assumption insures that the contribution $\tau_{\mathfrak{a}}\dot{\gamma}_{\mathfrak{a}} = |\tau_{\mathfrak{a}}||\dot{\gamma}_{\mathfrak{a}}| = |\tau_{\mathfrak{a}}|\dot{\nu}_{\mathfrak{a}}$ to the dissipation rate density remains greater than or equal to zero for all $\mathfrak{a} \in \{1,\ldots,m\}$. Such a constitutive assumption is made for other types of glide-system flow rules, e.g., the activation form

$$\dot{\gamma}_{\mathfrak{a}} = \dot{\gamma}_{\mathfrak{a}\,0}\,\exp\left\{-\frac{\Delta G_{\mathfrak{a}}(|\tau_{\mathfrak{a}}|,\,\tau_{\mathrm{C}\mathfrak{a}})}{k_{\mathrm{B}}\,\theta}\right\}\mathrm{sgn}(\tau_{\mathfrak{a}})$$

used by Anand et al. (1997) to model the inelastic behaviour of tantalum over a much wider range of strain rates and temperatures than possible with (92). Here, $\Delta G_{\mathfrak{a}}(|\tau_{\mathfrak{a}}|,\,\tau_{\mathrm{C}\mathfrak{a}})$ represents the activation Gibbs free energy for thermally-induced dislocation motion.

Consider next the dependence of $\dot{\rho}_{\mathrm{S}\mathfrak{a}}$ on $\dot{\gamma}_{\mathfrak{b}}$, i.e., $K_{\mathrm{S}\mathfrak{ab}}$. As it turns out, a number of existing approaches model this dependence. For example, in the approach of Estrin (1996, 1998) to dislocation-density-based constitutive modeling (see also * Estrin et al., 1998; Sluys and Estrin, 2000), this dependence follows from the constitutive relation

$$(93)\qquad \dot{\rho}_{\mathrm{S}\mathfrak{a}} = \left\{\sum_{\mathfrak{b}=1}^{n} j_{\mathrm{S}\mathfrak{ab}}\sqrt{\rho_{\mathrm{S}\mathfrak{b}}} - k_{\mathrm{S}\mathfrak{a}}\,\rho_{\mathrm{S}\mathfrak{a}}\right\}\mathrm{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\dot{\gamma}_{\mathfrak{a}}$$

*Because their model for SSD flux includes a Fickian-diffusion-like contribution due to dislocation cross-slip proportional to $\boldsymbol{n}_{\mathfrak{a}} \cdot \nabla\rho_{\mathrm{S}\mathfrak{a}}$, the approach of Sluys and Estrin (2000) does not fit into the current framework as it stands. The necessary extension involves treating the SSD densities ρ_{S} as, e.g., (independent) GIVs, analogous to the γ.

for the evolution of $\rho_{\mathrm{S}\mathfrak{a}}$ in terms of magnitude $|\dot\gamma_{\mathfrak{a}}| = \mathrm{sgn}(\dot\gamma_{\mathfrak{a}})\,\dot\gamma_{\mathfrak{a}}$ of $\dot\gamma_{\mathfrak{a}}$ for $\mathfrak{a} = 1, \ldots, m$. In (93), $j_{\mathrm{S}11}, j_{\mathrm{S}12}, \ldots$ represent the elements of the matrix of athermal dislocation storage coefficients, which in general are functions of ρ_{S}, and $k_{\mathfrak{a}}$ the glide-system coefficient of thermally-activated recovery. In this case, then,

$$I_{\mathrm{S}\mathfrak{ab}} = \delta_{\mathfrak{ab}} \left\{ \sum\nolimits_{\mathfrak{c}=1}^{n} j_{\mathrm{S}\mathfrak{bc}} \sqrt{\rho_{\mathrm{S}\mathfrak{c}}} - k_{\mathrm{S}\mathfrak{b}}\, \rho_{\mathrm{S}\mathfrak{b}} \right\}$$

holds, and so

$$(\boldsymbol{K}_{\mathrm{S}}^{\mathrm{T}} \psi_{\mathrm{D},\, \rho_{\mathrm{S}}})_{\mathfrak{a}} = K_{\mathrm{S}\mathfrak{aa}}\, \psi_{\mathrm{D},\, \rho_{\mathrm{S}\mathfrak{a}}} = \mathrm{sgn}(\dot\gamma_{\mathfrak{a}})\, I_{\mathrm{S}\mathfrak{aa}}\, \psi_{\mathrm{D},\, \rho_{\mathrm{S}\mathfrak{a}}}$$

from (91). Other such models for $K_{\mathrm{S}\mathfrak{ab}}$ can be obtained analogously from existing ones for $\dot\rho_{\mathrm{S}\mathfrak{a}}$ in the literature, e.g., from the dislocation-density-based approach of Teodosiu (1997).

Models such as those $(83)_2$ for $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$, or that (93) in the case of $\rho_{\mathrm{S}\mathfrak{a}}$, account in particular for dislocation-dislocation interactions. At least in these cases, then, such interactions are taken into account in the evolution relations for the dislocation measures, and so need not (necessarily) be accounted for in the form of ψ. From this point of view, ψ_{D} could take for example the simple "power-law" form

$$\begin{array}{rccccc} \psi_{\mathrm{D}} = & \frac{1}{2}\, \boldsymbol{E}_{\mathrm{E}} \cdot \mathcal{C}_{\mathrm{E}} \boldsymbol{E}_{\mathrm{E}} & + & s^{-1}\, c_{\mathrm{S}}\, \mu \sum\nolimits_{\mathfrak{a}=1}^{n} \epsilon_{\mathrm{S}\mathfrak{a}}^{2s} & + & g^{-1}\, c_{\mathrm{G}}\, \mu \sum\nolimits_{\mathfrak{a}=1}^{n} \epsilon_{\mathrm{G}\mathfrak{a}}^{2g} \\ =: & \psi_{\mathrm{DE}} & + & \psi_{\mathrm{DS}} & + & \psi_{\mathrm{DG}} \end{array} \tag{94}$$

in the case of ductile single crystals, perhaps the simplest possible. Here, $\mathcal{C}_{\mathrm{E}}$ represents the referential elasticity tensor, and

$$\boldsymbol{E}_{\mathrm{E}} := \tfrac{1}{2}(\boldsymbol{C}_{\mathrm{E}} - \boldsymbol{I})$$

the elastic Green strain determined by the corresponding right Cauchy-Green tensor

$$\boldsymbol{C}_{\mathrm{E}} := \boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}} \boldsymbol{C} \boldsymbol{F}_{\mathrm{P}}^{-1} \quad . \tag{95}$$

Further, c_{S} and c_{G} are (scaling) constants, s and g exponents, μ the average shear modulus, and

$$\begin{array}{rcl} \epsilon_{\mathrm{S}\mathfrak{a}} & := & \ell_{\mathrm{S}} \sqrt{\rho_{\mathrm{S}\mathfrak{a}}}\ , \\ \epsilon_{\mathrm{G}\mathfrak{a}} & := & \ell_{\mathrm{G}} \sqrt{|\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}|}\ , \end{array}$$

non-dimensional deformation-like internal variables associated with SSDs and GNDs, respectively, involving the characteristic lengths ℓ_{S} and ℓ_{G}, respectively. In particular, the GND contribution ψ_{DG} to ψ_{D} appearing in (94) is motivated by and represents a power-law generalization of the model of Kuhlmann-Wilsdorf (1989) for dislocation self-energy (see also Ortiz and Repetto, 1999) as based on the notion of dislocation line-length. From (94), we have in particular the simple expression

$$\tau_{\mathfrak{a}} = \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}} \cdot 2\, \boldsymbol{C}_{\mathrm{E}}\, \psi_{\mathrm{DE},\, \boldsymbol{C}_{\mathrm{E}}}$$

for the Schmid stress $\tau_{\mathfrak{a}}$ from (89) in terms of the Mandel stress $-\psi_{\mathrm{D},\, \boldsymbol{F}_{\mathrm{P}}} \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} = 2\, \boldsymbol{C}_{\mathrm{E}}\, \psi_{\mathrm{DE},\, \boldsymbol{C}_{\mathrm{E}}}$. In addition,

$$\begin{array}{rcl} \psi_{\mathrm{D},\, \rho_{\mathfrak{a}}} & = & c_{\mathrm{S}}\, \mu\, \ell_{\mathrm{S}}^{2s}\, \rho_{\mathrm{S}\mathfrak{a}}^{s-1}\ , \\ \psi_{\mathrm{D},\, \boldsymbol{g}_{\mathfrak{a}}} & = & c_{\mathrm{G}}\, \mu\, \ell_{\mathrm{G}}^{2g}\, |\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}|^{g-2}\, \boldsymbol{g}_{\mathrm{G}\mathfrak{a}}\ , \end{array}$$

then hold. From these, we obtain in turn

$$x_{\mathfrak{a}} = \begin{cases} 0 & \text{glide-system model} \\ c_{\mathrm{G}}\, \mu\, \ell_{\mathrm{G}}^{2g}\, |\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}|^{g-2} \sum\nolimits_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{g}_{\mathrm{G}\mathfrak{a}} \cdot \boldsymbol{g}_{\mathrm{G}\mathfrak{b}} & \text{continuum model} \end{cases} \tag{96}$$

from (90) for $x_{\mathfrak{a}}$,

$$(97)\qquad (\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{D},\,g_{\mathrm{G}}})_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,b^{-1}\,\ell_{\mathrm{G}}^{2g}\,|\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}|^{g-2}\begin{cases}\boldsymbol{n}_{\mathfrak{a}}\times\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} & \text{glide-system model}\\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}}\times\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} & \text{continuum model}\end{cases}$$

from (88), as well as the result

$$(98)\qquad r_{\mathfrak{a}} = c_{\mathrm{S}}\,\mu\,\ell_{\mathrm{S}}^{2s}\sum\nolimits_{\mathfrak{b}=1}^{m} I_{\mathrm{S}\mathfrak{b}\mathfrak{a}}\,\rho_{\mathrm{S}\mathfrak{b}}^{s-1}$$

from (91) for $r_{\mathfrak{a}}$. On the basis of models like that (93) of Estrin (1998) for $\dot{\rho}_{\mathrm{S}\mathfrak{a}}$, this last form for $r_{\mathfrak{a}}$ is consistent with and represents a generalization of distributed dislocation strength models (e.g., Kocks, 1976, 1987) to account for the effects of GNDs on glide-system (isotropic) hardening. Indeed, for $s = 1$, $r_{\mathfrak{a}}$ becomes proportional to $\sqrt{\rho_{\mathrm{S}\mathfrak{b}}}$ in the context of (93).

The simplest case of the formulation as based on (94) arises in the context of the glide-system model for GNDs when we set $s = 1$ and $g = 2$. Then

$$(99)\qquad (\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{D},\,g_{\mathrm{G}}})_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{4}\,b^{-1}\begin{cases} b^{-1}\boldsymbol{n}_{\mathfrak{a}}\times(\nabla\gamma_{\mathfrak{a}}\times\boldsymbol{n}_{\mathfrak{a}}) & \text{glide-system model}\\ \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}}\times\boldsymbol{g}_{\mathrm{G}\mathfrak{a}} & \text{continuum model}\end{cases}$$

follows from (87) for the flux contribution via (78) and (83). Note that $(99)_1$ follows from the fact that $(83)_1$ is integrable. Then, the corresponding reduction of $r_{\mathfrak{a}}$ from (98), (56) and $(99)_1$ implies in particular the evolution-field relation

$$(100)\qquad d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{4}\,b^{-2}\,\mathrm{div}_{\mathfrak{a}}(\nabla\gamma_{\mathfrak{a}}) + \tau_{\mathfrak{a}} - c_{\mathrm{S}}\,\mu\,\ell_{\mathrm{S}}^{2}\sum\nolimits_{\mathfrak{b}=1}^{m} K_{\mathrm{S}\mathfrak{b}\mathfrak{a}}$$

for $\gamma_{\mathfrak{a}}$ modeled as a GIV via (56), again in the context of the glide-system GND model, assuming c_{G}, μ and ℓ_{G} constant. The perhaps simplest possible non-trivial form of (100) for the evolution of $\gamma_{\mathfrak{a}}$ in the current context follows in particular from the corresponding simplest (i.e., quasi-linear) form* $d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}} = \beta_{\mathfrak{a}}\,\dot{\gamma}_{\mathfrak{a}}$ for $d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}}$ in terms of the glide-system damping modulus $\beta_{\mathfrak{a}} \geq 0$ with units of J s m^{-3} or Pa s (i.e., viscosity-like). In addition,

$$\mathrm{div}_{\mathfrak{a}}(\nabla\gamma_{\mathfrak{a}}) := (\boldsymbol{I} - \boldsymbol{n}_{\mathfrak{a}}\otimes\boldsymbol{n}_{\mathfrak{a}})\cdot\nabla(\nabla\gamma_{\mathfrak{a}}) = (\boldsymbol{s}_{\mathfrak{a}}\otimes\boldsymbol{s}_{\mathfrak{a}} + \boldsymbol{t}_{\mathfrak{a}}\otimes\boldsymbol{t}_{\mathfrak{a}})\cdot\nabla(\nabla\gamma_{\mathfrak{a}})$$

represents the projection of the divergence operator onto the glide plane spanned by $(\boldsymbol{s}_{\mathfrak{a}}, \boldsymbol{t}_{\mathfrak{a}})$. Given suitable forms for the constitutive quantities, then, the field relation (100) can in principal be solved (i.e., together with the momentum balance in the isothermal case) for $\gamma_{\mathfrak{a}}$. On the other hand, since $\boldsymbol{F}_{\mathrm{P}}$ does not depend explicitly on γ, and, in contrast to the glide-system model, $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ does not depend explicitly on γ and $\nabla\gamma$ in the continuum GND model, no "simple" expression like (100) for the evolution of $\gamma_{\mathfrak{a}}$ is obtainable in this case. Indeed, in all other cases, one must proceed more generally to solve initial-boundary-value problems for ξ, the γ, and θ. We return to this issue in the next section.

A second class of free energy models can be based on the choice $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \nu, \mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})$, i.e.,

$$(101)\qquad \psi(\theta, \boldsymbol{C}, \alpha) = \psi_{\mathrm{C}}(\theta, \boldsymbol{C}, \boldsymbol{F}_{\mathrm{P}}, \nu, \mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}) \quad ,$$

with

$$\dot{\nu}_{\mathfrak{a}} = |\dot{\gamma}_{\mathfrak{a}}|$$

*The coupling with ∇ in d_{V} and the dependence of d_{V} on $\nabla\dot{\gamma}_{\mathfrak{a}}$, is neglected here.

the glide-system accumulated slip rate. In this case, we have

$$(102)\qquad \begin{aligned}(K^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} &= -\tau_{\mathfrak{a}} + x_{\mathfrak{a}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\, r_{\mathfrak{a}}\ ,\\ (\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} &= \boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}} \times (\psi_{\mathrm{C,\,curl}\,\boldsymbol{F}_{\mathrm{P}}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}}\ ,\end{aligned}$$

via (26) and (89), where now

$$(103)\qquad x_{\mathfrak{a}} := \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}} \cdot \psi_{\mathrm{C,\,curl}\,\boldsymbol{F}_{\mathrm{P}}}(\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}}$$

and

$$r_{\mathfrak{a}} := \psi_{\mathrm{C},\,\nu_{\mathfrak{a}}}$$

Consider for example the particular form

$$(104)\qquad \begin{aligned}\psi_{\mathrm{C}} &= \tfrac{1}{2}\,\boldsymbol{E}_{\mathrm{E}}\cdot\mathcal{C}_{\mathrm{E}}\boldsymbol{E}_{\mathrm{E}} &+\quad \psi_{\mathrm{CS}}(\nu) &+\quad g^{-1}\,c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{g}\,|\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}|^{g}\\ &=: \quad\psi_{\mathrm{CE}} &+\quad \psi_{\mathrm{CS}} &+\quad \psi_{\mathrm{CG}}\end{aligned}$$

for ψ_{C} analogous to (94) for ψ_{D}. In this context, the choice

$$\psi_{\mathrm{CS}} = \frac{(\tau_S - \tau_0)^2}{h_0}\,\ln\left[\cosh\left(\frac{h_0}{\tau_S-\tau_0}\,\nu\right)\right]$$

yields the simple model for isotropic or Taylor hardening (i.e., due to SSDs) proposed by Hutchinson (1976), with

$$\nu := \sum\nolimits_{\mathfrak{a}=1}^{n} \nu_{\mathfrak{a}}$$

the total accumulated inelastic slip in all glide systems. Here, τ_S represents a characteristic saturation strength, τ_0 a characteristic initial critical resolved shear stress, and h_0 a characteristic initial hardening modulus, for all glide systems. Another possibility for ψ_{CS} is the form

$$\psi_{\mathrm{CS}} = \sum\nolimits_{\mathfrak{a}=1}^{n} r_{\mathfrak{a}0}\,\nu_{\mathfrak{a}} + s^{-1}\,h_0\,\nu^{s}$$

consistent with the model of Ortiz and Repetto (1999) for latent hardening in single crystals, with now

$$\nu := \sqrt{\sum\nolimits_{\mathfrak{a},\mathfrak{b}=1}^{n} \iota_{s\mathfrak{a}\mathfrak{b}}\,\nu_{\mathfrak{a}}\,\nu_{\mathfrak{b}}}$$

the effective total accumulated slip in all glide systems in terms of the interaction coefficients $\iota_{s\mathfrak{a}\mathfrak{b}}$, $\mathfrak{a}, \mathfrak{b} = 1, \ldots, n$. In particular, this model is based on the assumptions that (i), hardening is parabolic in single slip (i.e., for $s = 2/3$), and (ii), the hardening matrix $\psi_{\mathrm{CS},\,\nu_{\mathfrak{a}}\,\nu_{\mathfrak{b}}}$ is dominated by its off-diagonal components. Beyond such models for glide-system (isotropic) hardening, (104) yields the expression

$$x_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{g}\,|\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}|^{g-2}\,\boldsymbol{s}_{\mathfrak{a}}\otimes\boldsymbol{n}_{\mathfrak{a}}\cdot(\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})(\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}}$$

for glide-system back-stress from (103), as well as that

$$(\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha})_{\mathfrak{a}} = c_{\mathrm{G}}\,\mu\,\ell_{\mathrm{G}}^{g}\,|\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}}|^{g-2}\,\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}\boldsymbol{n}_{\mathfrak{a}}\times(\mathrm{curl}\,\boldsymbol{F}_{\mathrm{P}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}}$$

for $(\mathcal{J}_{\mathrm{G}}^{\mathrm{T}}\,\psi_{\mathrm{C,\,curl}\,\boldsymbol{F}_{\mathrm{P}}})_{\mathfrak{a}}$ from $(102)_2$. Analogous to $\boldsymbol{F}_{\mathrm{P}}$ and $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ in the case of the continuum GND model, because $\boldsymbol{F}_{\mathrm{P}}$ and curl $\boldsymbol{F}_{\mathrm{P}}$ do not depend explicitly on γ and $\nabla\gamma$, no field relation for $\gamma_{\mathfrak{a}}$ of the type (100) follows from (104), and we are again forced to proceed numerically.

8. The case of small deformation

Clearly, the formulation up to this point is valid for large deformation. For completeness, consider in this section the simplifications arising in the formulation under the assumption of small deformation. In particular, such a simplification is relevant to comparisons of the current approach with other modeling approaches such as the dislocation computer simulation of Van der Giessen and Needleman (1995). This has been carried out recently (Svendsen & Reese, 2002) in the context of the (isothermal) simple shear of a crystalline strip containing one or two glide planes. This model problem has been used in the recent work of Shu et al.(2001) in order to compare the predictions of the discrete dislocation computer simulation with those of the nonlocal strain-gradient approach of Fleck and Hutchinson (1997) and applied to crystal plasticity (e.g., Shu and Fleck, 1999). As dicusssed by them, it represents a model problem for the type of plastic constraint found at grain boundaries of a polycrystal, or the surface of a thin film, or at interfaces in a composite.

In the crystal plasticity context, the small-deformation formulation begins with the corresponding form

$$\boldsymbol{H}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{n} (\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}})\, \gamma_{\mathfrak{a}} \tag{105}$$

for the local inelastic displacement "gradient" $\boldsymbol{H}_{\mathrm{P}}$ assuming no initial inelastic deformation in the material. Note that this measure is in effect equivalent to the slip tensor $\gamma^{(I)} := \sum_{\mathfrak{a}=1}^{n} \gamma_{\mathfrak{a}}\, \boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}$ of Shizawa and Zbib (1999). In addition, note that $\boldsymbol{H}_{\mathrm{P}}$ can be considered as a function of γ in this case. In turn, (105) yields the expression

$$\operatorname{curl} \boldsymbol{H}_{\mathrm{P}} = \sum\nolimits_{\mathfrak{a}=1}^{n} \boldsymbol{s}_{\mathfrak{a}} \otimes (\nabla\gamma_{\mathfrak{a}} \times \boldsymbol{n}_{\mathfrak{a}}) \tag{106}$$

for the incompatibility of $\boldsymbol{H}_{\mathrm{P}}$. This is equivalent to the dislocation density tensor $\alpha^{(I)} := \operatorname{curl} \gamma^{(I)}$ of Shizawa and Zbib (1999). Note that either $\operatorname{curl} \boldsymbol{H}_{\mathrm{P}}$ or this latter measure may be considered a function of $\nabla\gamma$. In this context, then, rather than for example with the choice $(\boldsymbol{H}_{\mathrm{P}}, \nu, \operatorname{curl} \boldsymbol{H}_{\mathrm{P}})$, we could work alternatively with that $\alpha = (\gamma, \nu, \nabla\gamma)$ as a measure for the inelastic/dislocation state in the material at any material point $p \in B$. In fact, it would appear to be the simplest possible choice. Indeed, any such choice based alternatively on the small-deformation form

$$\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \begin{cases} b^{-1}\, \dot{\overline{\nabla\gamma_{\mathfrak{a}}}} \times \boldsymbol{n}_{\mathfrak{a}} & \text{glide-system model} \\ b^{-1}\, \dot{\overline{\nabla\gamma_{\mathfrak{a}}}} \times \boldsymbol{n}_{\mathfrak{a}} + \sum_{\mathfrak{b}\neq\mathfrak{a}} (\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\, \boldsymbol{g}_{\mathrm{G}\mathfrak{b}}\, \dot{\gamma}_{\mathfrak{a}} & \text{continuum model} \end{cases}$$

of (83) for the development of vector-valued glide-system GND density $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ would appear, at least in the context of the continuum model, to be more complicated since $\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}}$ is not exactly integrable, i.e., even in the small-strain case. On this basis, the general constitutive form (28) reduces to

$$\mathfrak{R} = \mathfrak{R}(\theta, \boldsymbol{E}, \gamma, \nu, \nabla\gamma, \nabla\theta, \dot{\gamma}, \nabla\dot{\gamma}, p)$$

for all dependent constitutive quantities (e.g., stress) in the small-deformation context, again with $\alpha = (\gamma, \nu, \nabla\gamma)$. Here,

$$\boldsymbol{E} := \operatorname{sym}(\nabla\boldsymbol{u})$$

represents the symmetric part of the displacement gradient. By analogy, the results of the thermodynamic formulations in §§4–5 for γ modeled as GIVs or as internal DOFs can used to obtain those for the case of small strain. Further, the reduced form (47) of ψ becomes

$$\psi = \psi(\theta, \boldsymbol{E}, \gamma, \nu, \nabla\gamma).$$

Consider for example the class

$$\psi(\theta, \boldsymbol{E}, \gamma, \nu, \nabla\gamma) = \psi_{\mathrm{C}}(\theta, \boldsymbol{E}, \boldsymbol{E}_{\mathrm{P}}(\gamma), \nu, \operatorname{curl} \boldsymbol{H}_{\mathrm{P}}(\nabla\gamma)) \tag{107}$$

of forms for ψ analogous to (101), with

$$\boldsymbol{E}_{\mathrm{P}} := \operatorname{sym}(\boldsymbol{H}_{\mathrm{P}}) \tag{108}$$

the inelastic strain. From (107) follow

$$\begin{aligned}
(K^{\mathrm{T}}\psi_{,\alpha})_{\mathfrak{a}} &= \psi_{,\gamma_{\mathfrak{a}}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{C},\,\nu_{\mathfrak{a}}} &&= -\tau_{\mathfrak{a}} + \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{C},\,\nu_{\mathfrak{a}}}\,,\\
(\mathcal{J}^{\mathrm{T}}\psi_{,\alpha})_{\mathfrak{a}} &= \psi_{,\nabla\gamma_{\mathfrak{a}}} &&= \boldsymbol{n}_{\mathfrak{a}} \times (\psi_{\mathrm{C},\,\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}}\,,
\end{aligned}$$

by analogy with (102) via (108) and (106), with now

$$\tau_{\mathfrak{a}} := -\,\boldsymbol{s}_{\mathfrak{a}} \cdot \psi_{\mathrm{C},\,\boldsymbol{E}_{\mathrm{P}}}\boldsymbol{n}_{\mathfrak{a}}$$

for the Schmid stress. In the case of small deformation, then, the contribution $x_{\mathfrak{a}}$ from inhomogeneity to the glide-system back stress vanishes identically. On the basis of these results, the form

$$d_{\mathrm{V},\,\dot{\gamma}_{\mathfrak{a}}} = \operatorname{div}[\boldsymbol{n}_{\mathfrak{a}} \times (\psi_{\mathrm{C},\,\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}})^{\mathrm{T}}\boldsymbol{s}_{\mathfrak{a}} + d_{\mathrm{V},\,\nabla\dot{\gamma}_{\mathfrak{a}}}] + \tau_{\mathfrak{a}} - \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{C},\,\nu_{\mathfrak{a}}} \tag{109}$$

of the evolution relation for the γ from (56) in the context of their modeling as GIVs, holds.

Further insight into (109) can be gained by introducing concrete forms for ψ_{C} and d_{V}. For example, consider that

$$\psi_{\mathrm{C}} = \tfrac{1}{2}\,\boldsymbol{E}_{\mathrm{E}} \cdot \mathcal{C}_{\mathrm{E}}\boldsymbol{E}_{\mathrm{E}} + \psi_{\mathrm{CS}}(\nu) + g^{-1}\mu\,\ell^{g}\,|\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}|^{g} \tag{110}$$

for ψ_{C} analogous to (104), with $\boldsymbol{E}_{\mathrm{E}} := \boldsymbol{E} - \boldsymbol{E}_{\mathrm{P}}$ now the (small) elastic strain, and $\boldsymbol{E}_{\mathrm{P}} := \operatorname{sym}(\boldsymbol{H}_{\mathrm{P}})$ the (small) inelastic strain. Further, the power-law form

$$d_{\mathrm{V}} = \frac{n}{n+1}\,\varsigma\,\dot{\nu}_0 \sum\nolimits_{\mathfrak{a}=1}^{m} \left\{\frac{|\dot{\gamma}_{\mathfrak{a}}|}{\dot{\nu}_0}\right\}^{(n+1)/n} \tag{111}$$

for the dissipation potential d_{V} is perhaps the simplest one for d_{V} of practical relevance. Here, ς represents a characteristic energy scale for activation of dislocation glide motion with units of J m^{-3} or Pa, and $\dot{\nu}_0$ a characteristic value of $|\dot{\gamma}_{\mathfrak{a}}|$. Substituting (110) and (111) into (109) results in the evolution/field relation

$$\varsigma\,\dot{\nu}_0^{-1}\dot{\gamma}_{\mathfrak{a}} = \mu\,\ell^2 \sum\nolimits_{\mathfrak{b}=1}^{m} \boldsymbol{A}_{\mathfrak{ab}} \cdot \nabla(\nabla\gamma_{\mathfrak{b}}) \;+\; \boldsymbol{s}_{\mathfrak{a}} \cdot (\mathcal{C}_{\mathrm{E}}\boldsymbol{E}_{\mathrm{E}})\boldsymbol{n}_{\mathfrak{a}} - \operatorname{sgn}(\dot{\gamma}_{\mathfrak{a}})\,\psi_{\mathrm{CS},\,\nu_{\mathfrak{a}}}$$

for the glide system slip $\gamma_{\mathfrak{a}}$ via the $g = 2$ and $n = 1$, with $\boldsymbol{A}_{\mathfrak{ab}} := (\boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,[(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{n}_{\mathfrak{b}})\,\boldsymbol{I} - \boldsymbol{n}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{b}}]$. In particular, note that $\boldsymbol{A}_{\mathfrak{aa}} \cdot \nabla(\nabla\gamma_{\mathfrak{a}}) = [\boldsymbol{I} - \boldsymbol{n}_{\mathfrak{a}} \otimes \boldsymbol{n}_{\mathfrak{a}}] \cdot \nabla(\nabla\gamma_{\mathfrak{a}}) = [\boldsymbol{s}_{\mathfrak{a}} \otimes \boldsymbol{s}_{\mathfrak{a}} + \boldsymbol{t}_{\mathfrak{a}} \otimes \boldsymbol{t}_{\mathfrak{a}}] \cdot \nabla(\nabla\gamma_{\mathfrak{a}})$ represents the divergence of $\nabla\gamma_{\mathfrak{a}}$ projected onto the $\mathfrak{a}^{\text{th}}$ glide plane. It is worth emphasizing that the form of this projection results from the dependence of ψ on $\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}$. For comparison, note that $\boldsymbol{A}_{\mathfrak{ab}} := (\boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{n}_{\mathfrak{b}})\boldsymbol{I}$, and so $\boldsymbol{A}_{\mathfrak{ab}} \cdot \nabla(\nabla\gamma_{\mathfrak{b}}) = (\boldsymbol{s}_{\mathfrak{a}} \cdot \boldsymbol{s}_{\mathfrak{b}})\,(\boldsymbol{n}_{\mathfrak{a}} \cdot \boldsymbol{n}_{\mathfrak{b}})\operatorname{div}(\nabla\gamma_{\mathfrak{b}})$, would hold if ψ depended on the inhomogeneity $\nabla\boldsymbol{H}_{\mathrm{P}}$ instead of on the incompatibility $\operatorname{curl}\boldsymbol{H}_{\mathrm{P}}$ of $\boldsymbol{H}_{\mathrm{P}}$. In the crystal plasticity and current context, at least, the distinction is significant in the sense that no additional hardening results in the current context when ψ depends directly on $\nabla\boldsymbol{H}_{\mathrm{P}}$.

9. Discussion

Consider the results of the two approaches to the modeling of the glide-system slips γ from §§4-5. Formally speaking, these differ in (i), the respective forms (56) and (72) for the evolution of the γ, (ii), those (55) and (71) for the rate of heating ω due to inelastic processes, and (iii), those (57) and $(68)_3$ for the heat flux density $\boldsymbol{q}$. In particular, in view of the corresponding forms (53) and (70) for temperature evolution, this latter difference is of no consequence for the field relations. Indeed, except for the contribution $\zeta_{\mathrm{F}\nabla\dot{\gamma}}$ to Φ_{N} in the internal DOF model for the γ, the total energy flux density $\boldsymbol{h}$ has the same form in both cases, i.e.,

$$
\begin{aligned}
\boldsymbol{h} &= -\boldsymbol{q} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi} = d_{\mathrm{V},\,\nabla\ln} + \zeta_{\mathrm{V}\,\nabla\ln} + (\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha} + d_{\mathrm{V},\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi}\ , \\
&= -\boldsymbol{q} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi} + \Phi_{\mathrm{F}}^{\mathrm{T}}\dot{\gamma} = d_{\mathrm{F},\,\nabla\ln} + \zeta_{\mathrm{F}\,\nabla\ln} + (\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha} + d_{\mathrm{F},\,\nabla\dot{\gamma}} + \zeta_{\mathrm{F}\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma} + \boldsymbol{P}^{\mathrm{T}}\dot{\xi}\ ,
\end{aligned}
$$

from $(30)_2$, (57), $(66)_1$ and $(68)_1$. This fact is related to the observation of Gurtin (1971, footnote 1) in the context of classical mixture theory concerning the interpretation of "entropy flux" and "heat flux" in phenomenology and the relation between these two. There, the issue was one of whether diffusion flux is to be interpreted as a flux of energy (e.g., Eckhart, 1940; Gurtin, 1971) or a flux of entropy (e.g., Meixner and Reik, 1959; DeGroot and Mazur, 1962; Müller, 1968). In the current context, the flux (density) of interest is that $(\mathcal{J}^{\mathrm{T}}\,\psi_{,\,\alpha} + d_{,\,\nabla\dot{\gamma}})^{\mathrm{T}}\dot{\gamma}$. In the GIV approach, the constitutive form (51) shows that this flux (i.e., divided by θ) is being interpreted as an entropy flux. On the other hand, $(58)_2$ and $(63)_2$ imply that it is being interpreted as an energy flux in the internal DOF approach. In this point, then, both approaches are consistent with each other.

As it turns out, the field relation (56) for the γ derived on the basis of the modeling of these as generalized internal variables, represents a generalized form of the Cahn-Allen field relation (e.g., Cahn, 1960; Cahn and Allen, 1977) for non-conservative phase fields, itself in turn a generalization of the Ginzburg-Landau model for phase transitions. In particular, (56) would reduce to the Cahn-Allen form (i), if d_{V} were proportional to a quadratic form in $\dot{\gamma}$ and independent of $\nabla\dot{\gamma}$, and (ii), if $\mathcal{J}^{\mathrm{T}}\psi_{,\,\alpha}$ and $K^{\mathrm{T}}\psi_{,\,\alpha}$ were reduceable to $\psi_{,\,\nabla\gamma}$ and $\psi_{,\,\gamma}$, respectively. In particular, this latter case arises only for monotonic loading and small deformation. The Cahn-Allen relation has been studied quite extensively from the mathematical point of view (see, e.g., Brokate and Sprekels, 1996). As such, one may profit from the corresponding literature on the solution of specific initial-boundary value problems in applications of the approach leading to (56), or more generally that leading to (72), which are currently in progress.

From a phenomenological point of view, the concrete form (94) for ψ_{D}, and in particular that of ψ_{DE}, or that of ψ_{CE} in (104), is contingent upon the modeling of $\boldsymbol{F}_{\mathrm{P}}$ as an elastic material isomorphism (e.g., Wang and Bloom, 1974; Bertram, 1993; Svendsen, 1998), i.e., inelastic processes represented by $\boldsymbol{F}_{\mathrm{P}}$ do not change the form of the elastic constitutive relation. Such an assumption, quite appropriate and basically universal for single-crystal plasticity, may be violated in the case of strong texture development, induced anisotropy and/or anisotropic damage in polycrystals. As discussed by Svendsen (1998), one consequence of the modeling of $\boldsymbol{F}_{\mathrm{P}}$ as an elastic isomorphism is the identification of

$$
\boldsymbol{F}_{\mathrm{E}} := \boldsymbol{F}\boldsymbol{F}_{\mathrm{P}}^{-1} \tag{112}
$$

as the local (elastic) deformation in the material, and in particular that of the crystal lattice in single-crystal plasticity. More generally, $\boldsymbol{F}_{\mathrm{P}}$ can be modeled as a material uniformity (Maugin and Epstein, 1998; Svendsen, 2001b) in the case of simple materials. In the current context,

(112) implies the connection

$$\operatorname{curl}^{\boldsymbol{F}_{\mathrm{P}}}\boldsymbol{F}_{\mathrm{E}} = -\det(\boldsymbol{F}_{\mathrm{P}}^{-1})\,\boldsymbol{F}_{\mathrm{E}}(\operatorname{curl}\boldsymbol{F}_{\mathrm{P}})\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}}$$

via (9) and (8) between incompatibility of the local lattice deformation $\boldsymbol{F}_{\mathrm{E}}$ with respect to the intermediate (local) "configuration" and that of $\boldsymbol{F}_{\mathrm{P}}$ with respect to the reference (local) "configuration" (i.e., placement) at each $p \in B$ via (10), (11), and the compatibility of $\boldsymbol{F}$. Alternatively, we have

$$\operatorname{curl}^{\boldsymbol{F}_{\mathrm{P}}}\boldsymbol{F}_{\mathrm{E}} = -\boldsymbol{F}_{\mathrm{E}}\,\boldsymbol{G}_{\mathrm{I}},$$

where*

$$\boldsymbol{G}_{\mathrm{I}} := \det(\boldsymbol{F}_{\mathrm{P}})^{-1}\,(\operatorname{curl}\boldsymbol{F}_{\mathrm{P}})\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} = \det(\boldsymbol{F}_{\mathrm{E}})\,(\operatorname{curl}^{\boldsymbol{F}}\boldsymbol{F}_{\mathrm{E}}^{-1})\boldsymbol{F}_{\mathrm{E}}^{-\mathrm{T}} \tag{113}$$

represents the geometric dislocation tensor recently introduced by Cermelli and Gurtin (2001). As shown by them, $\boldsymbol{G}_{\mathrm{I}}$ represents the incompatibility of $\boldsymbol{F}_{\mathrm{P}}$ relative to the surface element

$$\boldsymbol{n}_{\mathrm{I}}\,da_{\mathrm{I}} := \det(\boldsymbol{F}_{\mathrm{P}})\,\boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}}\boldsymbol{n}_S\,da_S$$

in the intermediate configuration. Indeed, relative to this element, the equivalence

$$(\operatorname{curl}\boldsymbol{F}_{\mathrm{P}})\boldsymbol{n}_S\,da_S = \boldsymbol{G}_{\mathrm{I}}\boldsymbol{n}_{\mathrm{I}}\,da_{\mathrm{I}}$$

holds. As such, curl $\boldsymbol{F}_{\mathrm{P}}$ gives the same measure of GNDs with respect to surface elements in the reference configuration as does $\boldsymbol{G}_{\mathrm{I}}$ with respect to such elements in the intermediate configuration. Note that $\boldsymbol{G}_{\mathrm{I}}$, like curl $\boldsymbol{F}_{\mathrm{P}}$, has units of inverse length. The definition $(113)_1$ implies the form

$$\dot{\boldsymbol{G}}_{\mathrm{I}} = \operatorname{curl}^{\boldsymbol{F}_{\mathrm{P}}}\boldsymbol{L}_{\mathrm{P}} + \boldsymbol{L}_{\mathrm{P}}\boldsymbol{G}_{\mathrm{I}} + \boldsymbol{G}_{\mathrm{I}}\boldsymbol{L}_{\mathrm{P}}^{\mathrm{T}} - \boldsymbol{G}_{\mathrm{I}}\,(\boldsymbol{I}\cdot\boldsymbol{L}_{\mathrm{P}}) \tag{114}$$

for the evolution of $\boldsymbol{G}_{\mathrm{I}}$ via (22). Alternatively, this can be expressed "objectively" as

$$\det(\boldsymbol{F}_{\mathrm{P}})^{-1}\,\boldsymbol{F}_{\mathrm{P}}\,\overline{[\det(\boldsymbol{F}_{\mathrm{P}})\,\boldsymbol{F}_{\mathrm{P}}^{-1}\boldsymbol{G}_{\mathrm{I}}\boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}}]}^{\,\cdot}\,\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} = \det(\boldsymbol{F}_{\mathrm{P}})^{-1}\,\boldsymbol{F}_{\mathrm{P}}\,\dot{\boldsymbol{G}}_{\mathrm{R}}\boldsymbol{F}_{\mathrm{P}}^{\mathrm{T}} = \operatorname{curl}^{\boldsymbol{F}_{\mathrm{P}}}\boldsymbol{L}_{\mathrm{P}} \tag{115}$$

relative to the "upper" Oldroyd-Truesdell derivative of $\boldsymbol{G}_{\mathrm{I}}$ with respect to $\boldsymbol{F}_{\mathrm{P}}$, where

$$\boldsymbol{G}_{\mathrm{R}} := \det(\boldsymbol{F}_{\mathrm{P}})\,\boldsymbol{F}_{\mathrm{P}}^{-1}\boldsymbol{G}_{\mathrm{I}}\boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}} = \boldsymbol{F}_{\mathrm{P}}^{-1}(\operatorname{curl}\boldsymbol{F}_{\mathrm{P}})$$

represents the referential form of $\boldsymbol{G}_{\mathrm{I}}$ via (113). In the current crystal plasticity context, the right-hand side of (115) reduces to

$$\operatorname{curl}^{\boldsymbol{F}_{\mathrm{P}}}\boldsymbol{L}_{\mathrm{P}} = b\sum\nolimits_{\mathfrak{a}=1}^{n}\boldsymbol{s}_{\mathfrak{a}}\otimes\boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}}\dot{\boldsymbol{g}}_{\mathrm{G}\mathfrak{a}} = \sum\nolimits_{\mathfrak{a}=1}^{n}\boldsymbol{s}_{\mathfrak{a}}\otimes\boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}}[\nabla\dot{\gamma}_{\mathfrak{a}}\times\boldsymbol{n}_{\mathfrak{a}}]$$

via (6) and (23) in terms of the evolution of the vector-valued GND surface density $\boldsymbol{g}_{\mathrm{G}\mathfrak{a}}$ for the glide-system GND model from (78). As such, (114) implies

$$\dot{\boldsymbol{G}}_{\mathrm{I}} = \sum\nolimits_{\mathfrak{a}=1}^{m}[(\boldsymbol{s}_{\mathfrak{a}}\otimes\boldsymbol{n}_{\mathfrak{a}})\boldsymbol{G}_{\mathrm{I}} + \boldsymbol{G}_{\mathrm{I}}(\boldsymbol{n}_{\mathfrak{a}}\otimes\boldsymbol{s}_{\mathfrak{a}})]\,\dot{\gamma}_{\mathfrak{a}} + \sum\nolimits_{\mathfrak{a}=1}^{m}\boldsymbol{s}_{\mathfrak{a}}\otimes\boldsymbol{F}_{\mathrm{P}}^{-\mathrm{T}}[\nabla\dot{\gamma}_{\mathfrak{a}}\times\boldsymbol{n}_{\mathfrak{a}}]$$

for the evolution of $\boldsymbol{G}_{\mathrm{I}}$ in the case of crystal plasticity via (23) and the fact that $\boldsymbol{I}\cdot\boldsymbol{L}_{\mathrm{P}} = 0$ in this context. So, another class of specific forms for ψ from (47) can be based on the choice $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \nu, \boldsymbol{G}_{\mathrm{I}}$, implying

$$\psi(\theta, \boldsymbol{C}, \alpha, p) = g(\theta, \boldsymbol{C}_{\mathrm{E}}, \nu, \boldsymbol{G}_{\mathrm{I}}, p)$$

*Recall that we have defined the curl of a second-order tensor field in (6) via $(\operatorname{curl}\boldsymbol{T})^{\mathrm{T}}\boldsymbol{a} := \operatorname{curl}(\boldsymbol{T}^{\mathrm{T}}\boldsymbol{a})$, rather than in the form $(\operatorname{curl}\boldsymbol{T})\boldsymbol{a} := \operatorname{curl}(\boldsymbol{T}^{\mathrm{T}}\boldsymbol{b})$ used by Cermelli and Gurtin (2001).

via (95). In turn, g itself is a member of the class defined by the choice $\alpha = (\boldsymbol{F}_{\mathrm{P}}, \nu, \nabla\boldsymbol{F}_{\mathrm{P}})$, as can be concluded directly from (25) and the fact that curl $\boldsymbol{F}_{\mathrm{P}}$ is a function of $\nabla\boldsymbol{F}_{\mathrm{P}}$ via (18). As shown by Cermelli and Gurtin (2001), constitutive functions for any $p \in B$ depending on $\nabla\boldsymbol{F}_{\mathrm{P}}$ must reduce to a dependence on $\boldsymbol{G}_{\mathrm{I}}$ for their form to be independent of change of compatible local reference placement at $p \in B$, i.e., one induced by a change* of global reference placement. This requirement is in turn based on the result of Davini (1986), and Davini and Parry (1989) that such changes leave dislocation measures such as $\boldsymbol{G}_{\mathrm{I}}$ unchanged, representing as such "elastic" changes of local reference placement. As it turns out, one can show more generally (Svendsen, 2001c) that ψ reduces to g for all $p \in B$, i.e., for B as a whole, under the assumption that $\boldsymbol{F}_{\mathrm{P}}$ represents a particular kind of material uniformity.

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*Since local changes of reference placement for any $p \in B$ represent equivalence classes of corresponding changes of global reference placement there, any local change of reference placement for $p \in B$ is induced by a corresponding change of global placement.

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