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by John D. Clayton, David L. McDowell, and Douglas J. Bammann

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14. ABSTRACT

Deformation mappings are considered that correspond to the motions of lattice defects, elastic stretch and rotation of the lattice, and initial defect distributions. Intermediate (i.e., relaxed) configuration spaces associated with these deformation maps are identified and then classified from the differential-geometric point of view. A fundamental issue is the proper selection of coordinate systems and metric tensors in these configurations when such configurations are classified as anholonomic. The particular choice of a global, external Cartesian coordinate system and corresponding covariant identity tensor as a metric on an intermediate configuration space is shown to be a constitutive assumption often made regardless of the existence of geometrically necessary crystal defects associated with the anholonomicity (i.e., the non-Euclidean nature) of the space. Since the metric tensor on the anholonomic configuration emerges necessarily in the definitions of scalar products, certain transpose maps, tensorial symmetry operations, and Jacobian invariants, its selection should not be trivialized. Several alternative (i.e., non-Euclidean) representations proposed in the literature for the metric tensor on anholonomic spaces are critically examined.

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Anholonomic configuration spaces and metric tensors in finite elastoplasticity

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Abstract

Deformation mappings are considered that correspond to the motions of lattice defects, elastic stretch and rotation of the lattice, and initial defect distributions. Intermediate (i.e., relaxed) configuration spaces associated with these deformation maps are identified and then classified from the differential-geometric point of view. A fundamental issue is the proper selection of coordinate systems and metric tensors in these configurations when such configurations are classified as anholonomic. The particular choice of a global, external Cartesian coordinate system and corresponding covariant identity tensor as a metric on an intermediate configuration space is shown to be a constitutive assumption often made regardless of the existence of geometrically necessary crystal defects associated with the anholonomicity (i.e., the non-Euclidean nature) of the space. Since the metric tensor on the anholonomic configuration emerges necessarily in the definitions of scalar products, certain transpose maps, tensorial symmetry operations, and Jacobian invariants, its selection should not be trivialized. Several alternative (i.e., non-Euclidean) representations proposed in the literature for the metric tensor on anholonomic spaces are critically examined.

Keywords: Elastoplasticity; Incompatibility; Configurations

1. Introduction

The notion of a relaxed "intermediate" or "natural" configuration in finite deformation anelasticity or elastoplasticity, wherein each local crystal volume element exhibits a stress-free state, was forwarded by many researchers in the mid-20th century [1–8]. Such a relaxed configuration may correspond to the intermediate configuration arising from the usual multiplicative decomposition of the deformation gradient [9,10], with the relaxed state associated with the local unloading of each volume element from its stressed state in the *current* (i.e., deformed or Eulerian) configuration. Alternatively, the relaxed configuration may correspond to local unloading of each volume element from its *reference* (i.e., initial or Lagrangian) state; such a natural configuration will differ from the initial configuration when the body contains a distribution of internal residual stress fields associated with crystal defects, for example [11,7,12].

It is important to note that in most cases the stress-free configuration is only locally coherent (i.e., simply connected or *holonomic*), since each volume element that undergoes relaxation will deform during

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the unloading process in a fashion that is incompatible with the relaxation deformations of its neighboring elements. In other words, a crystalline body supporting a distribution of heterogeneous internal stress fields associated with defects must generally be cut into multiple pieces in order to simultaneously relieve the stress in every piece. The ensemble of pieces comprises, in differential-geometric terminology, *an anholonomic space* [13,14], or a space that does not admit a *homeomorphism* (i.e., an invertible, bi-continuous, one-to-one mapping) to coordinates of a three-dimensional *Euclidean space*, the latter being the geometric space occupied by the coherent crystalline body prior to local stress relaxation. It is also understood stresses are relaxed to zero only in an average sense in the so-called "stress-free" configuration. In other words, when traction is removed from the external surface of each local volume element, self-equilibrating forces may still be present internally, within each element. Total relaxation of all internal forces (e.g., atomic and sub-atomic level interactions) can only be achieved at observation scales more far more refined than those describable by continuum elastoplasticity theories.

A well-known fact from differential geometry is that for a manifold (i.e., configuration space) to admit a single global Cartesian coordinate frame whose basis vectors are tangent to curves on the manifold, the space must be Euclidean [13,15]. Necessarily associated with the Euclidean property of the space is vanishing of the Riemann–Christoffel curvature tensor constructed from partial derivatives of the metric tensor of the coordinate system, with the metric tensor corresponding to the covariant identity tensor (i.e., a covariant Kronecker's delta) when a single Cartesian frame is selected. On the other hand, when the space is non-Euclidean (e.g., anholonomic), prescription of the Cartesian metric tensor implying a single set of three orthonormal basis vectors spanning the global anholonomic space may be an inappropriate assumption when such basis vectors are identified as tangents to the material manifold in the intermediate configuration [16]. In recognition of this issue, alternative covariant deformation measures (e.g., elastic, plastic, or total strain tensors) have been implemented as metric tensors for the purpose of lowering indices on contravariant quantities referred to anholonomic spaces [17–20].

In this work we first review the criteria for labeling a space as either holonomic or anholonomic and show how such spaces arise in finite elastoplasticity. We next demonstrate reasons why a metric tensor on the anholonomic configuration must often be specified: to define the transpose operation for mixed-variant tensors, to conduct symmetry operations on nominally mixed-variant tensors, to define Jacobian invariants of deformation mappings, and to define scalar products of vectors and contravariant tensors referred to the anholonomic space. Finally, several alternative choices for the anholonomic configuration coordinate system and associated metric tensor are presented and then critically evaluated within the context of finite elastoplasticity.

2. Anholonomic configurations in finite elastoplasticity

Consider the following multiplicative decompositions for the total deformation gradient $\mathbf{F}$ [21]:

$$\mathbf{F} = \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{p}} = \mathscr{K}\mathscr{K}_0^{-1},$$

$$F^a_{.A} = F^{\mathrm{e}^a}_{.\alpha} F^{\mathrm{p}^\alpha}_{.A} = \mathscr{K}^a_{.\alpha}\mathscr{K}_0^{-1^\alpha}{}_{.A}, \tag{1}$$

where the associated configurations and local tangent spaces are illustrated in Fig. 1, and where all indices

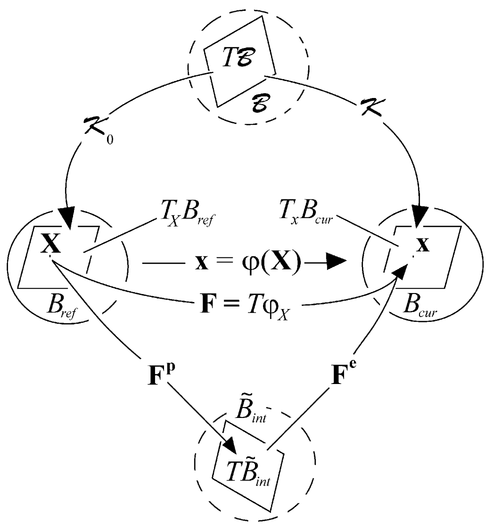

Fig. 1. Configurations and tangent maps.

$a, A, \alpha, \mathscr{a} = 1, 2, 3$. We label the *reference configuration* (i.e., the initial state) as B_{ref}, the *current configuration* (i.e., deformed state) as B_{cur}, the *intermediate configuration* of finite elastoplasticity (i.e., the relaxed state achieved via locally unloading from the current configuration) as $\tilde{B}_{\text{int}}$, and the *natural configuration* (i.e., the relaxed state achieved via local unloading from the reference configuration) as $\mathscr{B}$. Local unloading from the reference configuration is associated with relaxation of *internal* stress fields corresponding to dislocations and other defects present within the crystal(s) at the *initial* time, when the entire crystalline body is typically assumed to be free of *external* traction. Local unloading from the current configuration corresponds to simultaneous relaxation of internal stress fields due to dislocations and other defects present at the *current* time as well as any traction applied to the external surface of the crystalline body. As mentioned already, the particular relaxed configuration attained depends strongly upon the size of each local volume element, and the so-called "internal stress fields" that are relaxed here may be viewed as stresses arising from the traction applied externally to the surface of each local volume element. The elastic and plastic tangent maps of multiplicative elastoplasticity are written in Eq. (1) as $\mathbf{F}^{\text{e}}$ and $\mathbf{F}^{\text{p}}$, respectively. The tangent map $\mathscr{K}_0$ links the natural and reference configurations, while the tangent map $\mathscr{K}$ links the natural and current configurations. We remark that while some authors have multiplicatively decomposed our $\mathscr{K}$ into elastic and plastic parts [22,12], we find the decomposition (1) more convenient in the present setting, since in our approach the covariant leg of $\mathbf{F}^{\text{p}}$ is referred to the Euclidean space B_{ref}. In precise terms, when defined in terms of stress relaxation, the (inverse of the) elastic tangent map $\mathbf{F}^{\text{e}}$ is characterized only up to an arbitrary rotation tensor [10]. Some aspect of the microstructure is needed to specify the elastic (or plastic) rotation, such as local lattice orientation in classical crystal plasticity theories, for example (cf. [12]).

We require in the present work for $\mathbf{F}$ to be *compatible* (i.e., integrable, holonomic, or a *true* deformation gradient):

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}, \quad F^a_{.A} = \frac{\partial x^a}{\partial X^A}, \tag{2}$$

where $\mathbf{x}$ and $\mathbf{X}$ are current and reference coordinates, respectively, the former assumed to be smooth single-valued functions of the latter and time t. Following directly from (2), certain integrability conditions are automatically fulfilled:

$$\begin{aligned} F^a_{.A,B} &= \frac{\partial^2 x^a}{\partial X^A \partial X^B} = \frac{\partial^2 x^a}{\partial X^B \partial X^A} \\ &= F^a_{.B,A} \to F^a_{.A,B} - F^a_{.B,A} \equiv 2F^a_{.[A,B]} = 0, \end{aligned} \tag{3}$$

where, as shown, the subscripted comma denotes partial coordinate differentiation and the bracketed indices are anti-symmetrized.

In contrast to $\mathbf{F}$, the deformation maps $\mathbf{F}^{\text{e}}$, $\mathbf{F}^{\text{p}}$, $\mathscr{K}$, and $\mathscr{K}_0$ generally *do not* fulfill conditions analogous to (2) and (3); i.e., these maps are generally not integrable. In fact, the lack of their integrability is often associated with the presence of crystal defects (cf. [4,5]). For example, consider the line integral of the differential vector element $\mathrm{d}\tilde{\mathbf{x}} \equiv \mathbf{F}^{\text{p}}\,\mathrm{d}\mathbf{X}$ about a closed contour $\tilde{c}$ in $\tilde{B}_{\text{int}}$:

$$\begin{aligned} \tilde{b}^{\alpha} &\equiv \oint_{\tilde{c}} \mathrm{d}\tilde{x}^{\alpha} = \oint_{C} F^{\text{p}^{\alpha}}_{.A}\,\mathrm{d}X^A \\ &= -\int_A F^{\text{p}^{\alpha}}_{.[A,B]}\,\mathrm{d}X^A \wedge \mathrm{d}X^B, \end{aligned} \tag{4}$$

where we have assumed Cartesian coordinates $X^A \in B_{\text{ref}}$ and invoked Stokes' theorem (cf. [13,23]) to convert from a line integral to a surface integral over the area A enclosed by the loop C (the image of $\tilde{c}$ in B_{ref}), and where the skew-symmetric rank 2 differential area element is denoted by $\mathrm{d}X^A \wedge \mathrm{d}X^B$. In Eq. (4), $\tilde{\mathbf{b}}$ is typically called the *net Burgers vector* of all geometrically necessary dislocations piercing the area A at the current time. Equivalently, we may write for $\tilde{\mathbf{b}}$

$$\begin{aligned} \tilde{b}^{\alpha} &\equiv \oint_{\tilde{c}} \mathrm{d}\tilde{x}^{\alpha} = \oint_{c} F^{\text{e}-1^{\alpha}}_{.a}\,\mathrm{d}x^a \\ &= -\int_a F^{\text{e}-1^{\alpha}}_{.[a,b]}\,\mathrm{d}x^a \wedge \mathrm{d}x^b \end{aligned} \tag{5}$$

in terms of the inverse of the tangent map $\mathbf{F}^{\text{e}}$ and the area element $\mathrm{d}x^a \wedge \mathrm{d}x^b$ in the current configuration. We see from (5) that the anholonomicity of $\tilde{B}_{\text{int}}$ is directly related to defects present within the crystal at the *current time*, since configuration $\tilde{B}_{\text{int}}$ is defined in terms of local elastic unloading from B_{cur}. It should be noted that while Eq. (4) defines $\tilde{\mathbf{b}}$ in terms of differentiation and line and area elements referred to the reference configuration, $\tilde{\mathbf{b}}$ of (4) is equivalent to $\tilde{\mathbf{b}}$ of (5) and is *not* indicative of internal stress fields due to dislocations present at the *initial time*. Instead, we must define a different net Burgers vector $\mathscr{b}$ quantifying the anholonomicity of configuration $\mathscr{B}$ and representative of the defect densities present within the crystal at the initial time (since $\mathscr{B}$ is defined in terms of local elastic unloading from the initial state B_{ref}):

$$\mathscr{b}^{a} \equiv \oint_{c} \mathrm{d}\mathscr{x}^{a} = \oint_{c} \mathscr{K}^{-1^{a}}_{.a}\,\mathrm{d}x^{a}$$

$$= -\int_{a} \mathscr{K}^{-1^{a}}_{.[a,b]}\,\mathrm{d}x^{a} \wedge \mathrm{d}x^{b}, \tag{6}$$

$$\mathscr{b}^{a} \equiv \oint_{c} \mathrm{d}\mathscr{x}^{a} = \oint_{C} \mathscr{K}^{-1^{a}}_{0\ .A}\,\mathrm{d}X^{A}$$

$$= -\int_{A} \mathscr{K}^{-1^{a}}_{0\ .[A,B]}\,\mathrm{d}X^{A} \wedge \mathrm{d}X^{B}, \tag{7}$$

where c is a closed circuit in the natural configuration $\mathscr{B}$. In the interest of brevity, subsequent equations will focus upon the multiplicative decomposition $\mathbf{F}=\mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{p}}$ and the associated anholonomic space $\tilde{B}_{\text{int}}$; however, our arguments will generally also apply to the decomposition $\mathbf{F} = \mathscr{K}\mathscr{K}_{0}^{-1}$ and the corresponding anholonomic space $\mathscr{B}$.

Basis vectors locally tangent to the Euclidean spaces B_{ref} and B_{cur}, respectively, are written

$$\mathbf{G}_{A} \equiv \frac{\partial}{\partial X^{A}}, \quad \mathbf{g}_{a} \equiv \frac{\partial}{\partial x^{a}}. \tag{8}$$

Corresponding dual bases cotangent to B_{ref} and B_{cur}, respectively, are written as $\mathbf{G}^{A}$ and $\mathbf{g}^{a}$, and are defined such that the following dual (i.e., scalar) products are satisfied:

$$\langle \mathbf{G}^{A}, \mathbf{G}_{B}\rangle = \delta^{A}_{B}, \quad \langle \mathbf{g}^{a}, \mathbf{g}_{b}\rangle = \delta^{a}_{b}, \tag{9}$$

where δ^{A}_{B} and δ^{a}_{b} are Kronecker's delta symbols, i.e. $\delta^{A}_{B}=1$ for $A=B$, $\delta^{A}_{B}=0$ for $A\neq B$, with analogous relations for δ^{a}_{b}. From (8) we see that the basis vectors of the Euclidean spaces B_{ref} and B_{cur} are *holonomic basis vectors*, satisfying the integrability conditions [13]

$$\mathbf{G}_{[A,B]} = \mathbf{0}, \quad \mathbf{g}_{[a,b]} = \mathbf{0}. \tag{10}$$

The deformation gradient is then written as follows in terms of components and basis vectors:

$$\mathbf{F} = F^{a}_{.A}\mathbf{g}_{a} \otimes \mathbf{G}^{A} = \frac{\partial x^{a}}{\partial X^{A}}\,\mathbf{g}_{a} \otimes \mathbf{G}^{A}. \tag{11}$$

Similarly, we write for $\mathbf{F}^{\mathrm{e}}$ and $\mathbf{F}^{\mathrm{p}}$:

$$\mathbf{F}^{\mathrm{p}} = F^{\mathrm{p}^{\alpha}}_{.A}\tilde{\mathbf{g}}_{\alpha} \otimes \mathbf{G}^{A}, \quad \mathbf{F}^{\mathrm{e}} = F^{\mathrm{e}^{a}}_{.\alpha}\mathbf{g}_{a} \otimes \tilde{\mathbf{g}}^{\alpha}, \tag{12}$$

where the *anholonomic basis vectors* $\tilde{\mathbf{g}}_{\alpha}$ and associated covectors $\tilde{\mathbf{g}}^{\alpha}$ must obey

$$\langle \tilde{\mathbf{g}}^{\alpha}, \tilde{\mathbf{g}}_{\beta}\rangle = \delta^{\alpha}_{\beta} \tag{13}$$

in order to ensure satisfaction of the multiplicative decomposition (1), and where $\delta^{\alpha}_{\beta}=1$ for $\alpha=\beta$ and $\delta^{\alpha}_{\beta}=0$ for $\alpha\neq\beta$. In general, $\tilde{\mathbf{g}}_{[\alpha,\beta]} \neq \mathbf{0}$ (compare with Eq. (10) for holonomic bases), since we cannot differentiate with respect to *anholonomic coordinates* $\tilde{x}^{\alpha} \in \tilde{B}_{\text{int}}$ in the conventional manner and since no relations analogous to (8) apply to the $\tilde{\mathbf{g}}_{\alpha}$. If we *define* anholonomic coordinate differentiation as [13]

$$\frac{\partial(\,)}{\partial \tilde{x}^{\alpha}} \equiv \frac{\partial(\,)}{\partial X^{A}}F^{\mathrm{p}-1^{A}}_{.\alpha} = \frac{\partial(\,)}{\partial x^{a}}F^{\mathrm{e}^{a}}_{.\alpha}, \tag{14}$$

then

$$\tilde{\mathbf{g}}_{[\alpha,\beta]} = \tilde{\mathbf{g}}_{[\alpha,A}F^{\mathrm{p}-1^{A}}_{.\beta]} = \tilde{\mathbf{g}}_{[\alpha,a}F^{\mathrm{e}^{a}}_{.\beta]} \neq 0 \tag{15}$$

are additional conditions associated with the anholonomicity of configuration $\tilde{B}_{\text{int}}$. On the other hand, *only when $\tilde{B}_{\text{int}}$ is simply connected (and Euclidean)*, meaning that the $\tilde{x}^{\alpha}$ are holonomic coordinates of x^{a} or X^{A}, do we have

$$F^{\mathrm{p}^{\alpha}}_{.A} = \frac{\partial \tilde{x}^{\alpha}}{\partial X^{A}}, \quad F^{\mathrm{e}-1^{\alpha}}_{.a} = \frac{\partial \tilde{x}^{\alpha}}{\partial x^{a}}, \quad \tilde{\mathbf{g}}_{\alpha} = \frac{\partial}{\partial \tilde{x}^{\alpha}},$$

$$\tilde{\mathbf{g}}_{[\alpha,\beta]} = \mathbf{0}. \tag{16}$$

3. The metric tensor on an anholonomic space

The metric tensor on the anholonomic space $\tilde{B}_{\text{int}}$ is written here as $\tilde{\mathbf{g}} = \tilde{g}_{\alpha\beta}\tilde{\mathbf{g}}^{\alpha} \otimes \tilde{\mathbf{g}}^{\beta}$ and is symmetric by definition, i.e. $\tilde{g}_{\alpha\beta} = \tilde{g}_{\beta\alpha}$. It satisfies

$$\tilde{g}_{\alpha\beta} = \tilde{\mathbf{g}}_{\alpha} \cdot \tilde{\mathbf{g}}_{\beta}, \tag{17}$$

where "·" denotes the scalar product or inner product of contravariant vectors. The scalar product of two arbitrary vectors $\tilde{\mathbf{a}}$ and $\tilde{\mathbf{b}}$ on the tangent space of $\tilde{B}_{\text{int}}$ then becomes, from (17),

$$\tilde{\mathbf{a}} \cdot \tilde{\mathbf{b}} = \tilde{a}^{\alpha}\tilde{\mathbf{g}}_{\alpha} \cdot \tilde{b}^{\beta}\tilde{\mathbf{g}}_{\beta} = \tilde{a}^{\alpha}\tilde{b}^{\beta}(\tilde{\mathbf{g}}_{\alpha} \cdot \tilde{\mathbf{g}}_{\beta}) = \tilde{a}^{\alpha}\tilde{g}_{\alpha\beta}\tilde{b}^{\beta}. \tag{18}$$

Components of the metric tensor $\tilde{\mathbf{g}}$ are used to lower indices in the conventional manner, i.e.,

$$\tilde{a}_\alpha = \tilde{g}_{\alpha\beta}\tilde{a}^\beta, \tag{19}$$

and are needed to compute the transpose maps of mixed-variant tensors (cf. [15]), e.g.,

$$F^{\mathrm{e}T^\alpha}_{.a} = \tilde{g}^{\alpha\beta}F^{\mathrm{e}^b}_{.\beta}g_{ab} = \tilde{g}^{\alpha\beta}F^{\mathrm{e}^*\ .b}_{\beta}g_{ba},$$

$$F^{\mathrm{p}T^A}_{.\alpha} = \tilde{g}_{\alpha\beta}F^{\mathrm{p}^\beta}_{.B}G^{AB} = \tilde{g}_{\alpha\beta}F^{\mathrm{p}^*\ .\beta}_{B}G^{BA}, \tag{20}$$

where $\tilde{g}^{\alpha\beta}$ are components of the inverse metric $\tilde{\mathbf{g}}^{-1}$, G^{AB} are components of the inverse of the metric tensor $\mathbf{G}$ on the reference configuration B_{ref}, and g_{ab} are components of the metric tensor $\mathbf{g}$ on B_{cur}. Additionally in (20) the dual map operation corresponding to a horizontal exchange of indices is denoted by the superposed "$*$" [24,25]. From relations (20), we are in position to define symmetric elastic and plastic strain tensors referred to the current and reference configurations, respectively, e.g. the covariant $\mathbf{C}^{\mathrm{e}}$ and $\mathbf{C}^{\mathrm{p}}$:

$$C^{\mathrm{e}}_{ab} \equiv F^{\mathrm{e}T^\alpha}_{.a}g_{bc}F^{\mathrm{e}^c}_{.\alpha} = C^{\mathrm{e}}_{ba},$$

$$C^{\mathrm{p}}_{AB} \equiv F^{\mathrm{p}T^C}_{.\alpha}G_{CA}F^{\mathrm{p}^\alpha}_{.B} = C^{\mathrm{p}}_{BA}. \tag{21}$$

The metric tensor $\tilde{\mathbf{g}}$ is also needed to symmetrize nominally mixed-variant tensors referred to configuration $\tilde{B}_{\mathrm{int}}$. For example, consider the so-called "plastic velocity gradient" $\tilde{\mathbf{L}}^{\mathrm{p}}$:

$$\tilde{\mathbf{L}}^{\mathrm{p}} \equiv \dot{\mathbf{F}}^{\mathrm{p}}\mathbf{F}^{\mathrm{p}-1}, \quad \tilde{L}^{\mathrm{p}^\alpha}_{.\beta} \equiv \dot{F}^{\mathrm{p}^\alpha}_{.A}F^{\mathrm{p}-1^A}_{.\beta}, \tag{22}$$

where the superposed dot denotes the material time derivative. The transpose of the *covariant* version of $\tilde{\mathbf{L}}^{\mathrm{p}}$ is written

$$\tilde{L}^{\mathrm{p}T}_{\alpha\beta} = \tilde{L}^{\mathrm{p}}_{\beta\alpha} = \tilde{g}_{\beta\chi}\dot{F}^{\mathrm{p}^\chi}_{.A}F^{\mathrm{p}-1^A}_{.\alpha} \tag{23}$$

from which follow the *covariant* symmetric rate of plastic deformation $\tilde{\mathbf{D}}^{\mathrm{p}}$ and the skew-symmetric "plastic spin" $\tilde{\mathbf{W}}^{\mathrm{p}}$:

$$2\tilde{D}^{\mathrm{p}}_{\alpha\beta} = \tilde{L}^{\mathrm{p}}_{\alpha\beta} + \tilde{L}^{\mathrm{p}}_{\beta\alpha}, \quad 2\tilde{W}^{\mathrm{p}}_{\alpha\beta} = \tilde{L}^{\mathrm{p}}_{\alpha\beta} - \tilde{L}^{\mathrm{p}}_{\beta\alpha},$$

$$\tilde{L}^{\mathrm{p}}_{\alpha\beta} = \tilde{D}^{\mathrm{p}}_{\alpha\beta} + \tilde{W}^{\mathrm{p}}_{\alpha\beta}. \tag{24}$$

Multiplying (24) by through by $\tilde{g}^{\alpha\beta}$ results in

$$\tilde{L}^{\mathrm{p}^\alpha}_{.\beta} = \tilde{g}^{\alpha\chi}\tilde{D}^{\mathrm{p}}_{\chi\beta} + \tilde{g}^{\alpha\chi}\tilde{W}^{\mathrm{p}}_{\chi\beta} = \tilde{D}^{\mathrm{p}^\alpha}_{.\beta} + \tilde{W}^{\mathrm{p}^\alpha}_{.\beta}, \tag{25}$$

where $\tilde{D}^{\mathrm{p}^\alpha}_{.\beta} \equiv \tilde{g}^{\alpha\chi}\tilde{D}^{\mathrm{p}}_{\chi\beta}$ and $\tilde{W}^{\mathrm{p}^\alpha}_{.\beta} \equiv \tilde{g}^{\alpha\chi}\tilde{W}^{\mathrm{p}}_{\chi\beta}$ both depend upon the metric $\tilde{\mathbf{g}}$ (from (23)) and its inverse (from (25)). We thus see that the plastic velocity gradient $\tilde{\mathbf{L}}^{\mathrm{p}}$ can only be decomposed into stretch rate and spin terms after a metric tensor $\tilde{\mathbf{g}}$ has been introduced, as noted by Maugin [18].

Jacobian invariants of deformation mappings $\mathbf{F}^{\mathrm{e}}$ and $\mathbf{F}^{\mathrm{p}}$ defining the relationships between volume elements $\mathrm{d}v \subset B_{\mathrm{cur}}$, $\mathrm{d}\tilde{v} \subset \tilde{B}_{\mathrm{int}}$, and $\mathrm{d}V \subset B_{\mathrm{ref}}$ also depend upon $\tilde{\mathbf{g}}$. For example, letting $\tilde{z}^\alpha$ and Z^A denote coordinates referred to local Cartesian frames on $\tilde{B}_{\mathrm{int}}$ and B_{ref}, respectively, we write [8]

$$J^{\mathrm{p}} \equiv \frac{\mathrm{d}\tilde{v}}{\mathrm{d}V} = \det\left(\frac{\partial\tilde{z}^\alpha}{\partial Z^A}\right) = \det\left(\frac{\partial\tilde{z}^\alpha}{\partial\tilde{x}^\beta}F^{\mathrm{p}^\beta}_{.B}\frac{\partial X^B}{\partial Z^A}\right)$$

$$= \det(F^{\mathrm{p}^\beta}_{.B})\sqrt{\det(\tilde{g}_{\alpha\beta})/\det(G_{AB})}, \tag{26}$$

where we have used the identities $\det(\tilde{g}_{\alpha\beta}) = (\det(\partial\tilde{z}^\alpha/\partial\tilde{x}^\beta))^2$ and $\det(G_{AB}) = (\det(\partial Z^A/\partial X^B))^2$ (cf. [15]). Analogously for $\mathbf{F}^{\mathrm{e}}$ we write

$$J^{\mathrm{e}} \equiv \frac{\mathrm{d}v}{\mathrm{d}\tilde{v}} = \det\left(\frac{\partial z^a}{\partial\tilde{z}^\alpha}\right) = \det\left(\frac{\partial z^a}{\partial x^b}F^{\mathrm{e}^b}_{.\beta}\frac{\partial\tilde{x}^\beta}{\partial\tilde{z}^\alpha}\right)$$

$$= \det(F^{\mathrm{e}^b}_{.\beta})\sqrt{\det(g_{ab})/\det(\tilde{g}_{\alpha\beta})}, \tag{27}$$

with z^a denoting Cartesian coordinates on B_{cur} such that $\det(g_{ab}) = (\det(\partial z^a/\partial x^b))^2$. We can alternatively write (26) and (27) as [26]

$$J^{\mathrm{p}} = \tfrac{1}{6}\tilde{\varepsilon}_{\alpha\beta\chi}\varepsilon^{ABC}F^{\mathrm{p}^\alpha}_{.A}F^{\mathrm{p}^\beta}_{.B}F^{\mathrm{p}^\chi}_{.C}$$

$$= \tfrac{1}{6}(\sqrt{\tilde{g}/G})e_{\alpha\beta\chi}e^{ABC}F^{\mathrm{p}^\alpha}_{.A}F^{\mathrm{p}^\beta}_{.B}F^{\mathrm{p}^\chi}_{.C}, \tag{28}$$

$$J^{\mathrm{e}} = \tfrac{1}{6}\tilde{\varepsilon}^{\alpha\beta\chi}\varepsilon_{abc}F^{\mathrm{e}^a}_{.\alpha}F^{\mathrm{e}^b}_{.\beta}F^{\mathrm{e}^c}_{.\chi}$$

$$= \tfrac{1}{6}(\sqrt{g/\tilde{g}})e^{\alpha\beta\chi}e_{abc}F^{\mathrm{e}^a}_{.\alpha}F^{\mathrm{e}^b}_{.\beta}F^{\mathrm{e}^c}_{.\chi}, \tag{29}$$

where we have used the shorthand notation $g \equiv \det(g_{ab})$, $\tilde{g} \equiv \det(\tilde{g}_{\alpha\beta})$, and $G \equiv \det(G_{AB})$. Permutation *tensors* in Eqs. (28) and (29) are defined by $\varepsilon^{ABC} \equiv \sqrt[-1]{G}e^{ABC}$, $\tilde{\varepsilon}_{\alpha\beta\chi} \equiv \sqrt{\tilde{g}}e_{\alpha\beta\chi}$, $\varepsilon_{abc} \equiv \sqrt{g}e_{abc}$, and $\tilde{\varepsilon}^{\alpha\beta\chi} \equiv \sqrt[-1]{\tilde{g}}e^{\alpha\beta\chi}$, with e^{ABC}, $e_{\alpha\beta\chi}$, e_{abc}, and $e^{\alpha\beta\chi}$ standard permutation *symbols* each referred to the configuration indicated by its indices. Consider for example the incompatibility described by Eq. (5), which can be rewritten as

$$\tilde{b}^\alpha = -\int_a F^{\mathrm{e}-1^\alpha}_{.[a,b]}\,\mathrm{d}x^a \wedge \mathrm{d}x^b = -\int_a \varepsilon^{abc}F^{\mathrm{e}-1^\alpha}_{.[a,b]}n_c\,\mathrm{d}a$$

$$= -\int_a \varepsilon^{abc}F^{\mathrm{e}-1^\alpha}_{.a,b}n_c\,\mathrm{d}a = \int_a A^{\mathrm{e}^{\alpha c}}n_c\,\mathrm{d}a, \tag{30}$$

where the second rank area element has been converted to an axial covector $\mathbf{n}\,\mathrm{d}a$ via $\mathrm{d}x^a \wedge \mathrm{d}x^b = \varepsilon^{abc} n_c\,\mathrm{d}a$, and where the two-point dislocation density tensor $A^{\mathrm{e}^{\alpha c}} \equiv -\varepsilon^{abc} F^{\mathrm{e}-1^{\alpha}}_{.a,b}$. Mapping the integrand in (30) to the intermediate configuration via Nanson's formula (cf. [27]) gives

$$\tilde{b}^{\alpha} = \int_a A^{\mathrm{e}^{\alpha c}} n_c\,\mathrm{d}a = \int_{\tilde{a}} J^{\mathrm{e}} F^{\mathrm{e}-1^{\beta}}_{.c} A^{\mathrm{e}^{\alpha c}} \tilde{n}_{\beta}\,\mathrm{d}\tilde{a} = \int_{\tilde{a}} \tilde{A}^{\mathrm{e}^{\beta\alpha}} \tilde{n}_{\beta}\,\mathrm{d}\tilde{a}, \tag{31}$$

where $\tilde{A}^{\mathrm{e}^{\beta\alpha}} \equiv J^{\mathrm{e}} F^{\mathrm{e}-1^{\beta}}_{.c} A^{\mathrm{e}^{\alpha c}}$ is the intermediate configuration dislocation density tensor, which depends upon J^{e} and hence, from Eq. (29), $\tilde{g}$. Should we opt to allow the (scalar) residual free energy $\tilde{\psi}^{\mathrm{GN}}$ of the crystal associated with geometrically necessary dislocations to depend quadratically upon a dislocation density measure referred to $\tilde{B}_{\mathrm{int}}$ such as $\tilde{\mathbf{A}}^{\mathrm{e}}$ (cf. [27–29]), we then write, for example,

$$\tilde{\psi}^{\mathrm{GN}} = \tfrac{1}{2}\mu l^2 \tilde{\mathbf{A}}^{\mathrm{e}} : \tilde{\mathbf{A}}^{\mathrm{e}} = \tfrac{1}{2}\mu l^2 \tilde{A}^{\mathrm{e}^{\alpha\beta}} \tilde{g}_{\alpha\chi} \tilde{g}_{\beta\delta} \tilde{A}^{\mathrm{e}^{\chi\delta}}, \tag{32}$$

where μ and l are an elastic shear modulus and characteristic length, respectively. Thus, the scalar product in Eq. (32) is another instance in finite crystalline elastoplasticity where $\tilde{\mathbf{g}}$ is required.

4. Metric tensors and anholonomic basis vectors: possible choices

We now discuss some conceivable choices for the metric tensor $\tilde{\mathbf{g}}$ and associated basis vectors $\tilde{\mathbf{g}}_{\alpha}$. The simplest and by far most prevalent option from the literature is to impose (cf. [7,8,22,30])

$$\tilde{g}_{\alpha\beta} = \tilde{\mathbf{g}}_{\alpha} \cdot \tilde{\mathbf{g}}_{\beta} = \delta_{\alpha\beta}, \tag{33}$$

with $\delta_{\alpha\beta}$ the covariant Kronecker's delta, i.e. $\delta_{\alpha\beta} = 1$ for $\alpha = \beta$ and $\delta_{\alpha\beta} = 0$ for $\alpha \neq \beta$. Eq. (33) indicates that contravariant vectors defined on $\tilde{B}_{\mathrm{int}}$ are referred to a single global Cartesian frame (i.e., orthonormal $\tilde{\mathbf{g}}_{\alpha}$), or, equivalently, a parallel (i.e., identical) Cartesian frame attached to each local relaxed volume element $\mathrm{d}\tilde{v} \subset \tilde{B}_{\mathrm{int}}$. Such a choice implies either that (i) $\tilde{B}_{\mathrm{int}}$ is a Euclidean space or that (ii) the $\tilde{\mathbf{g}}_{\alpha}$ are not actually tangent to any coordinate lines scribed on the base manifold $\tilde{B}_{\mathrm{int}}$ (since such coordinates do not exist in the discontinuous anholonomic space) but instead correspond to some external reference frame. As discussed already in Section 2 of the present work, statement (i) is ruled out in the presence of crystal defects such as dislocations that render $\tilde{B}_{\mathrm{int}}$ anholonomic. This leaves statement (ii), which is difficult to interpret geometrically: from its standpoint, vectors in configuration $\tilde{B}_{\mathrm{int}}$ are not referred to the actual tangent spaces of a material manifold in $\tilde{B}_{\mathrm{int}}$ but are instead referred to the fixed external Cartesian frame(s). The intermediate metric $\delta_{\alpha\beta}$ (or equivalently, the external Cartesian frame) is introduced rather artificially in such theories as an additional constitutive entity, accompanying variables $\mathbf{F}^{\mathrm{e}}$ and $\mathbf{F}^{\mathrm{p}}$. We also mention the related work of Simo [31], wherein the intermediate configuration metric is given by $\tilde{g}_{\alpha\beta} = \delta^{A}_{.\alpha} G_{AB} \delta^{B}_{.\beta}$, implying a Euclidean metric structure for $\tilde{B}_{\mathrm{int}}$ when B_{ref} is Euclidean, and relying upon the external two-point construct $\delta^{A}_{.\alpha}$. While we are unable to rigorously rule out the choice (33) on any fundamental grounds, we emphasize next several alternatives that have been proposed in the literature that, in contrast to Eq. (33), do *not* make the embedding of a *non-Euclidean space* $\tilde{B}_{\mathrm{int}}$ within a global Cartesian space equipped with a *Euclidean metric tensor* $\delta_{\alpha\beta}$. (It should be noted, however, that our derivations (26) and (27), wherein Cartesian $\tilde{z}^{\alpha}$ are assigned to each volume element $\mathrm{d}\tilde{v} \subset \tilde{B}_{\mathrm{int}}$, *do* rely on such an assumption, at least locally.)

One such alternative is to specify the metric tensor $\tilde{\mathbf{g}}$ as the covariant elastic deformation tensor $\tilde{\mathbf{C}}^{\mathrm{e}}$ [17,18,20], i.e.

$$\tilde{g}_{\alpha\beta} = \tilde{C}^{\mathrm{e}}_{\alpha\beta} \equiv F^{\mathrm{e}^{a}}_{.\alpha} g_{ab} F^{\mathrm{e}^{b}}_{.\beta} = F^{\mathrm{e}^{a}}_{.\alpha} \mathbf{g}_a \cdot F^{\mathrm{e}^{b}}_{.\beta} \mathbf{g}_b = \tilde{\mathbf{g}}_{\alpha} \cdot \tilde{\mathbf{g}}_{\beta}, \tag{34}$$

implying that the anholonomic basis vectors are defined by $\tilde{\mathbf{g}}_{\alpha} \equiv F^{\mathrm{e}^{a}}_{.\alpha} \mathbf{g}_a$. Analogously, one could implement the covariant plastic deformation tensor $\tilde{\mathbf{C}}^{\mathrm{p}}$ as a metric [32]

$$\tilde{g}_{\alpha\beta} = \tilde{C}^{\mathrm{p}}_{\alpha\beta} \equiv F^{\mathrm{p}-1^{A}}_{.\alpha} G_{AB} F^{\mathrm{p}-1^{B}}_{.\beta} = F^{\mathrm{p}-1^{A}}_{.\alpha} \mathbf{G}_A \cdot F^{\mathrm{p}-1^{B}}_{.\beta} \mathbf{G}_B = \tilde{\mathbf{g}}_{\alpha} \cdot \tilde{\mathbf{g}}_{\beta}, \tag{35}$$

meaning that $\tilde{\mathbf{g}}_{\alpha} \equiv F^{\mathrm{p}-1^{A}}_{.\alpha} \mathbf{G}_A$. (It should be noted that Miehe [32] suggested several alternative metric tensors on each configuration, in addition to (35).) In Eqs. (34) and (35) we have used, respectively, the standard Euclidean relations $g_{ab} = \mathbf{g}_a \cdot \mathbf{g}_b$ and $G_{AB} = \mathbf{G}_A \cdot \mathbf{G}_B$. The $\tilde{\mathbf{g}}_{\alpha}$ in (34) or (35) are still not tangent to any global coordinate curves $\tilde{x}^\alpha$ (since such coordinates are precluded by the anholonomicity of $\tilde{B}_{\rm int}$), but they do exist in a one-to-one manner with the set $\mathbf{g}_a(\mathbf{x})$ and the map $\mathbf{F}^{\rm e}$ or with the set $\mathbf{G}_A(\mathbf{X})$ and the map $\mathbf{F}^{\rm p-1}$, respectively. It follows that $\tilde{\mathbf{C}}^{\rm e}$ and $\tilde{\mathbf{C}}^{\rm p}$ are well-defined geometric quantities referred to the space $\tilde{B}_{\rm int}$, in contrast to the somewhat artificial, external object $\delta_{\alpha\beta}$ of (33) that cannot be derived from the elastic or plastic tangent maps and basis vectors on $B_{\rm ref}$ or $B_{\rm cur}$. Consider now the rank 4 Riemann–Christoffel curvature tensor formed from $\tilde{\mathbf{C}}^{\rm e}$ on the anholonomic space $\tilde{B}_{\rm int}$, with components [13,14]

$$\tilde{R}^{\alpha}_{\beta\chi\delta} \equiv \frac{\partial\tilde{\Gamma}^{\alpha}_{\delta\beta}}{\partial\tilde{x}^{\chi}} - \frac{\partial\tilde{\Gamma}^{\alpha}_{\chi\beta}}{\partial\tilde{x}^{\delta}} + \tilde{\Gamma}^{\alpha}_{\chi\varepsilon}\tilde{\Gamma}^{\varepsilon}_{\delta\beta} - \tilde{\Gamma}^{\alpha}_{\delta\varepsilon}\tilde{\Gamma}^{\varepsilon}_{\chi\beta} + 2\tilde{\kappa}^{\varepsilon}_{\chi\delta}\tilde{\Gamma}^{\alpha}_{\varepsilon\beta}, \tag{36}$$

where the coefficients of the metric connection are found by $2\tilde{C}^{\rm e}_{\alpha\beta}\tilde{\Gamma}^{\alpha}_{\delta\chi} = \tilde{C}^{\rm e}_{\chi\beta,\delta} + \tilde{C}^{\rm e}_{\delta\beta,\chi} - \tilde{C}^{\rm e}_{\delta\chi,\beta}$ and components of the anholonomic object by $\tilde{\kappa}^{\varepsilon}_{\chi\delta} = F^{{\rm e}^a}_{.\chi}F^{{\rm e}^b}_{.\delta}F^{{\rm e}-1^\varepsilon}_{.[a,b]}$. The conditions $\tilde{R}^{\alpha}_{\beta\chi\delta} = 0$ and $\tilde{\kappa}^{\varepsilon}_{\chi\delta} = 0$ hold identically only when $F^{{\rm e}^a}_{.\alpha} = x^a_{,\alpha}$, i.e., only when $\tilde{B}_{\rm int}$ is homeomorphic to the Euclidean space $B_{\rm cur}$ and $\tilde{x}^\alpha$ are holonomic coordinates for which we can define partial differentiation as usual. Under such conditions, $\tilde{R}^{\alpha}_{\beta\chi\delta}$ is the pull-back of the curvature tensor formed from the metric tensor g_{ab}, which itself vanishes since $B_{\rm cur}$ is Euclidean. Analogous statements regarding the curvature can be made for $\tilde{\mathbf{C}}^{\rm p}$, i.e. the curvature tensor derived from $\tilde{\mathbf{C}}^{\rm p}$ vanishes identically only when $F^{{\rm p}^\alpha}_{.A} = \tilde{x}^{\alpha}_{,A}$ and $\tilde{B}_{\rm int}$ is Euclidean.

A third alternative methodology [33] involves introduction of the new multiplicative decomposition

$$\mathbf{F} = \hat{\mathbf{F}}^{\rm e}\hat{\mathbf{F}}^{\rm p}, \quad F^{a}_{.A} = \hat{F}^{{\rm e}^a}_{.B}\hat{F}^{{\rm p}^B}_{.A}, \tag{37}$$

where both legs of the new plastic deformation tensor $\hat{\mathbf{F}}^{\rm p}$ are referred to $B_{\rm ref}$ and where $\hat{\mathbf{F}}^{\rm e}$ is a two-point tensor between tangent spaces of $B_{\rm ref}$ and $B_{\rm cur}$, i.e.

$$\hat{\mathbf{F}}^{\rm e} = \hat{F}^{{\rm e}^a}_{.B}\mathbf{g}_a \otimes \mathbf{G}^B, \quad \hat{\mathbf{F}}^{\rm p} = \hat{F}^{{\rm p}^B}_{.A}\mathbf{G}_B \otimes \mathbf{G}^A. \tag{38}$$

Following Le and Stumpf [33], we introduce the two-point transformation matrix $\mathbf{H}$, satisfying

$$F^{{\rm e}^a}_{.\alpha} = \hat{F}^{{\rm e}^a}_{.B}H^{-1^B}_{.\alpha}, \quad F^{{\rm p}^\alpha}_{.A} = H^{\alpha}_{.B}\hat{F}^{{\rm p}^B}_{.A}, \tag{39}$$

such that Eqs. (1) and (37) are satisfied simultaneously

$$F^{a}_{.A} = F^{{\rm e}^a}_{.\alpha}F^{{\rm p}^\alpha}_{.A} = \hat{F}^{{\rm e}^a}_{.B}H^{-1^B}_{.\alpha}H^{\alpha}_{.B}\hat{F}^{{\rm p}^B}_{.A} = \hat{F}^{{\rm e}^a}_{.B}\hat{F}^{{\rm p}^B}_{.A}. \tag{40}$$

The anholonomic basis vectors and covectors are found in terms of $\mathbf{H}$ as, respectively,

$$\tilde{\mathbf{g}}_\alpha \equiv H^{-1^A}_{.\alpha}\mathbf{G}_A, \quad \tilde{\mathbf{g}}^\alpha \equiv H^{\alpha}_{.A}\mathbf{G}^A, \tag{41}$$

so that the dual product obeys the standard relations

$$\langle\tilde{\mathbf{g}}_\alpha, \tilde{\mathbf{g}}^\beta\rangle = \langle H^{-1^A}_{.\alpha}\mathbf{G}_A, H^{\beta}_{.B}\mathbf{G}^B\rangle = H^{-1^A}_{.\alpha}H^{\beta}_{.B}\langle\mathbf{G}_A, \mathbf{G}^B\rangle = H^{-1^A}_{.\alpha}H^{\beta}_{.B}\delta^B_A = \delta^\beta_\alpha, \tag{42}$$

leading then to the representation of the metric tensor on $\tilde{B}_{\rm int}$:

$$\tilde{g}_{\alpha\beta} = \tilde{\mathbf{g}}_\alpha \cdot \tilde{\mathbf{g}}_\beta = H^{-1^A}_{.\alpha}\mathbf{G}_A \cdot H^{-1^B}_{.\beta}\mathbf{G}_B = H^{-1^A}_{.\alpha}G_{AB}H^{-1^B}_{.\beta}. \tag{43}$$

Eq. (41) implies that the elastic deformation maps $\mathbf{F}^{\rm e}$ and $\hat{\mathbf{F}}^{\rm e}$ are the same (two-point) tensor, although each is referred to different coordinate bases:

$$\mathbf{F}^{\rm e} = F^{{\rm e}^a}_{.\alpha}\mathbf{g}_a \otimes \tilde{\mathbf{g}}^\alpha = (\hat{F}^{{\rm e}^a}_{.C}H^{-1^C}_{.\alpha})\mathbf{g}_a \otimes (H^{\alpha}_{.B}\mathbf{G}^B) = \hat{F}^{{\rm e}^a}_{.B}\mathbf{g}_a \otimes \mathbf{G}^B = \hat{\mathbf{F}}^{\rm e}. \tag{44}$$

Analogously, for the plastic tangent mappings we have

$$\mathbf{F}^{\rm p} = F^{{\rm p}^\alpha}_{.A}\tilde{\mathbf{g}}_\alpha \otimes \mathbf{G}^A = (\hat{F}^{{\rm p}^C}_{.A}H^{\alpha}_{.C})(H^{-1^B}_{.\alpha}\mathbf{G}_B) \otimes \mathbf{G}^A = \hat{F}^{{\rm p}^B}_{.A}\mathbf{G}_B \otimes \mathbf{G}^A = \hat{\mathbf{F}}^{\rm p}. \tag{45}$$

From the anholonomicity conditions (15) we see that

$$\tilde{\mathbf{g}}_{[\alpha,\beta]} = H^{-1^A}_{.[\alpha,\beta]}\mathbf{G}_A + H^{-1^A}_{.[\alpha}\mathbf{G}_{A,\beta]} = H^{-1^A}_{.[\alpha,\beta]}\mathbf{G}_A + H^{-1^A}_{.[\alpha}\mathbf{G}_{A,B}F^{{\rm p}-1^B}_{.\beta]} \neq \mathbf{0}. \tag{46}$$

Upon choosing a Cartesian reference coordinate system for the Euclidean space $B_{\rm ref}$, we obtain $\mathbf{G}_{A,B} = \mathbf{0}$, and Eq. (46) becomes

$$\tilde{\mathbf{g}}_{[\alpha,\beta]} = H^{-1^A}_{.[\alpha,\beta]}\mathbf{G}_A \neq \mathbf{0} \to H^{-1^A}_{.[\alpha,\beta]} \neq 0, \tag{47}$$

meaning that $\mathbf{H}$ (or its inverse) is generally not derivable as the gradient of a vector-valued function when $\tilde{B}_{\rm int}$ is anholonomic. On the other hand, *only when the intermediate configuration is holonomic* and $\tilde{\mathbf{g}}_{[\alpha,\beta]} = \mathbf{0}$ can we write

$$H^{\alpha}_{.A} = \frac{\partial\tilde{y}^{\alpha}}{\partial X^A}, \quad H^{-1^A}_{.\alpha} = \frac{\partial X^A}{\partial\tilde{y}^{\alpha}}, \tag{48}$$

where $\tilde{y}^{\alpha} = \tilde{y}^{\alpha}(X^A, t)$ are new coordinate functions on $\tilde{B}_{\mathrm{int}}$, not necessarily identical to $\tilde{x}^{\alpha}$. Upon invocation of the holonomicity relations (16) we obtain

$$\hat{F}^{\mathrm{e}^a}_{\cdot A} = F^{\mathrm{e}^a}_{\cdot\alpha} \frac{\partial \tilde{y}^{\alpha}}{\partial X^A} = \frac{\partial x^a}{\partial \tilde{x}^{\alpha}} \frac{\partial \tilde{y}^{\alpha}}{\partial X^A},$$

$$\hat{F}^{\mathrm{p}^B}_{\cdot A} = \frac{\partial X^B}{\partial \tilde{y}^{\alpha}} F^{\mathrm{p}^{\alpha}}_{\cdot A} = \frac{\partial X^B}{\partial \tilde{y}^{\alpha}} \frac{\partial \tilde{x}^{\alpha}}{\partial X^A}, \tag{49}$$

from which, for the particular choice of $\tilde{x}^{\alpha} = \tilde{y}^{\alpha}$, results in $\hat{F}^{\mathrm{e}^a}_{\cdot A} = F^a_{\cdot A}$ and $\hat{F}^{\mathrm{p}^B}_{\cdot A} = \delta^B_{\cdot A}$. Returning now to the anholonomic case and substituting (39) into (4), we see that the incompatibility (i.e., closure failure or net Burgers vector in configuration $\tilde{B}_{\mathrm{int}}$) depends simultaneously upon gradients of $\hat{F}^{\mathrm{p}^B}_{\cdot A}$ and $H^{\alpha}_{\cdot C}$:

$$\begin{aligned}\tilde{b}^{\alpha} &= -\int_A (H\hat{F}^{\mathrm{p}})^{\alpha}_{\cdot[A,B]}\, \mathrm{d}X^A \wedge \mathrm{d}X^B \\ &= -\int_A (\hat{F}^{\mathrm{p}^C}_{\cdot[A,B]} H^{\alpha}_{\cdot C} + \hat{F}^{\mathrm{p}^C}_{\cdot[A} H^{\alpha}_{\cdot C,B]})\, \mathrm{d}X^A \wedge \mathrm{d}X^B,\end{aligned} \tag{50}$$

implying that knowledge of components and gradients of $\hat{F}^{\mathrm{p}^B}_{\cdot A}$ alone is not sufficient to characterize the incompatibility of Eq. (4) (i.e., one needs either $F^{\mathrm{p}^{\alpha}}_{\cdot A}$ (Eq. (4)), $F^{\mathrm{e}-1^{\alpha}}_{\cdot a}$ (Eq. (5)), or *both* of $\hat{F}^{\mathrm{p}^B}_{\cdot A}$ and $H^{\alpha}_{\cdot B}$ (Eq. (50)). Thus, while attractive at first glance since no anholonomic basis vectors directly enter the multiplicative decomposition (37), the methodology outlined in Eqs. (37)–(50) can only be used within the context of *classical* higher-order gradient, dislocation-based crystalline elastoplasticity, wherein the incompatibility is referred to the anholonomic *intermediate* configuration $\tilde{B}_{\mathrm{int}}$, when the additional tensor $\mathbf{H}$ and its inverse are available for mapping to and from that configuration. However, the method should definitely not be disregarded, as Le and Stumpf [33] successfully applied this description to define a different Burgers vector $\mathbf{B}$ (i.e., an incompatibility) referred to the holonomic *reference* configuration, in terms of the lack of integrability of $\hat{\mathbf{F}}^{\mathrm{e}}$, i.e.

$$B^A \equiv \oint_c \hat{F}^{\mathrm{e}-1^A}_{\cdot a}\, \mathrm{d}x^a = -\int_a \hat{F}^{\mathrm{e}-1^A}_{\cdot[a,b]}\, \mathrm{d}x^a \wedge \mathrm{d}x^b. \tag{51}$$

It should be noted that in this context, components of $\hat{F}^{\mathrm{e}^a}_{\cdot A}$ are not associated with loading from a locally unstressed and anholonomic state to a stressed state, but rather describe, at each point in the crystal, the stretch and rotation of a triad of lattice director vectors occurring between the initial configuration and the current configuration, with $\hat{\mathbf{F}}^{\mathrm{p}} = \hat{\mathbf{F}}^{\mathrm{e}-1}\mathbf{F}$ any remaining "inelastic" deformation referred to the reference state.

5. Discussion

Additional critical comments regarding the particular choices of intermediate configuration metric tensor listed in Eqs. (33), (34), (35), and (43) are now in order. Consider first the designation given by (33): $\tilde{g}_{\alpha\beta} = \delta_{\alpha\beta}$. This prescription is by far the most common in finite deformation plasticity theories from the literature, as it is made implicitly whenever Cartesian coordinates for the intermediate configuration $\tilde{B}_{\mathrm{int}}$ are invoked, be it for the purpose of defining differential volume change [7,8], calculating a norm or scalar product of contravariant vectors or tensors [27–30], or decomposing the plastic velocity gradient $\tilde{\mathbf{L}}^{\mathrm{p}}$ into distinct deformation rate and spin terms (cf. [34]). We remark that Regueiro et al. [29] acknowledged the non-Euclidean character of $\tilde{B}_{\mathrm{int}}$ but gave no explicit alternative to the Cartesian metric tensor for use on $\tilde{B}_{\mathrm{int}}$. As stated already, choice (33) cannot be ruled out unequivocally via mathematical or physical arguments. However, since the unit metric tensor (i.e., covariant Kronecker's delta $\delta_{\alpha\beta}$) is not considered a well-defined *geometric variable* on a non-Euclidean space (cf. [16]), and since $\tilde{B}_{\mathrm{int}}$ is clearly non-Euclidean (i.e., not homeomorphic to three-dimensional Euclidean space) under conditions of heterogeneous, incompatible plastic deformation, the metric $\delta_{\alpha\beta}$ of (33) must be viewed as an additional, stationary *constitutive variable* introduced by the modeler, accompanying any constitutive relations specifying the time evolution of components of $\mathbf{F}^{\mathrm{e}}$ and $\mathbf{F}^{\mathrm{p}}$. In contrast, the choices given in (34), (35), and (43)—wherein the intermediate metric tensors are defined directly in terms of elastic or inelastic tangent mappings—may be viewed as favorable alternatives to (33) since the former do *not* require the modeler to prescribe an intermediate metric via introduction of an additional constitutive variable. Maugin [19] voiced similar opinions regarding the choice of metric tensor on our natural configuration $\mathscr{B}$ (Fig. 1), cautioning against usage of a Cartesian metric on a non-Euclidean space. Instead, Maugin [19] elected to employ the quantity $\mathscr{K}^a_{\cdot\alpha} g_{ab} \mathscr{K}^b_{\cdot\beta}$ as a metric for lowering contravariant indices on the generally anholonomic space $\mathscr{B}$. It should also be noted that while the *covariant* object $\delta_{\alpha\beta}$ cannot be constructed directly from anholonomic mappings $\mathbf{F}^{\mathrm{e}}$ or $\mathbf{F}^{\mathrm{p}}$, the *mixed-variant* unit tensor (i.e., *true* Kronecker's delta) $\delta^{\alpha}_{.\beta}$ can be introduced explicitly via the inverse operation, i.e. $\delta^{\alpha}_{.\beta} = F^{\mathrm{e}-1^{\alpha}}_{.a} F^{\mathrm{e}^{a}}_{.\beta}$ or $\delta^{\alpha}_{.\beta} = F^{\mathrm{p}^{\alpha}}_{.A} F^{\mathrm{p}-1^{A}}_{.\beta}$.

Eq. (34), prescribing $\tilde{g}_{\alpha\beta} = \tilde{C}^{\mathrm{e}}_{\alpha\beta} \equiv F^{\mathrm{e}^{a}}_{.\alpha} g_{ab} F^{\mathrm{e}^{b}}_{.\beta}$ as a possible alternative to (33), has been proposed explicitly by at least several others [17,18,20], and is analogous to the aforementioned approach favored by Maugin [19] when $\mathscr{K}$ is replaced by $\mathbf{F}^{\mathrm{e}}$. The quantity $\tilde{C}^{\mathrm{e}}_{\alpha\beta}$ is considered to be a well-defined geometric entity with indices referred to the intermediate configuration $\tilde{B}_{\mathrm{int}}$, since its constituents $F^{\mathrm{e}^{a}}_{.\alpha}$ and g_{ab} are by definition single-valued functions of current coordinates x^{a}. (This is in contrast to the external construct $\delta_{\alpha\beta}$ which must be introduced by an additional constitutive assumption.) Moreover, the Riemann–Christoffel curvature tensor $\tilde{R}^{\alpha}_{\beta\chi\delta}$ and the anholonomic object $\kappa^{\alpha}_{\beta\chi}$ of Eq. (36) both vanish identically only when $\mathbf{F}^{\mathrm{e}-1}$ is an integrable function of $\mathbf{x}$ and $\tilde{B}_{\mathrm{int}}$ is Euclidean, meaning that assignment of $\tilde{C}^{\mathrm{e}}_{\alpha\beta}$ as components of a metric tensor agrees fully with the non-Euclidean nature of the generally anholonomic space $\tilde{B}_{\mathrm{int}}$. Consider also the implications of choice (34) in a thermodynamic assumption for stored elastic energy such as Eq. (32): the free energy associated with geometrically necessary dislocations, written herein as $\tilde{\psi}^{\mathrm{GN}}$, would depend explicitly upon the elastic strain metric $\tilde{C}^{\mathrm{e}}_{\alpha\beta}$. Such an assumption is in fact supported by previous physical [35] and numerical [36] experiments on various ductile pure metals and their alloys, wherein amplification of internal energy of dislocation arrays at flexing grain and sub-grain boundaries in the presence of applied loads was discovered. In light of the above reasons, we endorse here usage of $\tilde{C}^{\mathrm{e}}_{\alpha\beta}$ as a viable alternative to $\delta_{\alpha\beta}$ as a metric tensor on the globally non-Euclidean, anholonomic space $\tilde{B}_{\mathrm{int}}$.

Prescription of the plastic strain tensor $\tilde{C}^{\mathrm{p}}_{\alpha\beta} \equiv F^{\mathrm{p}-1^{A}}_{.\alpha} G_{AB} F^{\mathrm{p}-1^{B}}_{.\beta}$ as a metric $\tilde{g}_{\alpha\beta}$ was suggested in Eq. (35), following previous work by Miehe [32]. The quantity $\tilde{C}^{\mathrm{p}}_{\alpha\beta}$ is considered to be a well-defined geometric entity with indices referred to the intermediate configuration, since its constituents $F^{\mathrm{p}-1^{A}}_{.\alpha}$ and G_{AB} are by definition single-valued functions of reference coordinates X^{A} and time t. This approach appears especially attractive since for the case of no plastic deformation (and hence no defects or anholonomicity), we have $F^{\mathrm{p}-1^{A}}_{.\alpha} = \delta^{A}_{.\alpha}$ and $\tilde{g}_{\alpha\beta} = \delta^{A}_{.\alpha} G_{AB} \delta^{B}_{.\beta}$, thus reducing to the prescription of Simo [31]. However, from the perspective of Eq. (32), this method presents some difficulties, since the plastic strain $\tilde{C}^{\mathrm{p}}_{\alpha\beta}$ would enter the free energy expression $\tilde{\psi}^{\mathrm{GN}}$, and since we do not view the plastic strain in most cases as a useful state quantity or accurate measure of stored elastic energy. The latter point is of no concern in local theories (e.g. Miehe [32]) wherein higher-order deformation gradients are not explicitly considered and energetic quantities such as $\tilde{\psi}^{\mathrm{GN}}$ of (32) are not computed. But in nonlocal thermomechanical theories framed in the relaxed intermediate configuration (cf. [27–29]) wherein relations such as (32) are invoked, then we regard the choice of intermediate metric $\tilde{C}^{\mathrm{e}}_{\alpha\beta}$ (34) as more physically plausible than the choice $\tilde{g}_{\alpha\beta} = \tilde{C}^{\mathrm{p}}_{\alpha\beta}$ (35).

Finally, consider the aforementioned approach of Le and Stumpf [33], with the multiplicative decomposition in component form given by Eq. (37): $F^{a}_{.A} = \hat{F}^{\mathrm{e}^{a}}_{.B} \hat{F}^{\mathrm{p}^{B}}_{.A}$. As discussed already, this decomposition enjoys the simplicity of not requiring any anholonomic basis vectors or corresponding intermediate metric tensor. Moreover, this method offers an alternative viewpoint of kinematics of elastic deformation in terms of the total deformation (between B_{ref} and B_{cur}) of a triad of lattice director vectors assigned to each material point. However, as we have shown in Eq. (50), quantification of the anholonomicity of $\tilde{B}_{\mathrm{int}}$ (i.e., the lack of integrability of $F^{\mathrm{p}^{\alpha}}_{.A}$) requires knowledge of the anholonomic mapping $\mathbf{H}$, which in turn implies the intermediate configuration metric $\tilde{g}_{\alpha\beta} = H^{-1^{A}}_{.\alpha} G_{AB} H^{-1^{B}}_{.\beta}$ as noted in Eq. (43). (It should be mentioned that the metric $H^{-1^{A}}_{.\alpha} G_{AB} H^{-1^{B}}_{.\beta}$ is generally non-Euclidean, so this choice does not contradict the non-Euclidean nature of the anholonomic space $\tilde{B}_{\mathrm{int}}$.) From the perspective of Eq. (50), since $H^{\alpha}_{.B}$ and its gradient are required, *in addition* to $\hat{F}^{\mathrm{p}^{B}}_{.A}$ and its gradient, this method is more complicated than the other choices (34) and (35), which require only higher gradients of either $F^{\mathrm{p}^{\alpha}}_{.A}$ (Eq. (4)) or $F^{\mathrm{e}-1^{\alpha}}_{.a}$ (Eq. (5)). This aspect leads us to favor $\tilde{g}_{\alpha\beta} = \tilde{C}^{\mathrm{e}}_{\alpha\beta}$ (34) over $\tilde{g}_{\alpha\beta} = H^{-1^{A}}_{.\alpha} G_{AB} H^{-1^{B}}_{.\beta}$ (43).

6. Concluding remarks

In higher-order gradient plasticity theories couched explicitly upon the mechanics of incompatible defects, special care should be taken when prescribing metric tensors for the anholonomic (e.g., natural or intermediate) configurations that are inherent to the kinematic description, since various scalar products, transpose maps, tensorial symmetry operations, and Jacobian invariants depend explicitly upon the chosen anholonomic basis vectors and their inner product. We discuss several alternative choices to the popular and apparently contradictory (but not incorrect) choice of a Euclidean metric tensor (and accompanying Cartesian basis vectors) attached to an anholonomic (and hence non-Euclidean) configuration space. Endorsed here as an intermediate configuration metric is the pull-back of the current configuration metric tensor by the elastic deformation mapping (i.e., the covariant elastic strain referred to the intermediate configuration).

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