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**On the Evolution of Plasticity and Incompatibility**

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*Dedicated to the memory of Ronald Rivlin*

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*Abstract:* The phenomenological theory of elastic-plastic deformations is reconsidered in the light of recent opinion regarding the constitutive character of their constituent elastic and plastic components. The primary role of dissipation in the physics of plastic evolution is emphasized and shown to lead to the clarification of a number of open questions. Particular attention is given to the invariance properties of the elastic and plastic deformations, to the kinematics of discontinuities, and to the role of material symmetry in restricting constitutive equations for elastic response, yield and plastic evolution.

## 1. Introduction

The modern literature on the phenomenological theory of metal plasticity emphasizes a multiplicative decomposition of the deformation gradient into elastic and plastic factors in which the former measures distortion relative to some unstressed or *relaxed* configuration of a local neighborhood of a material point. The definition of the elastic deformation in terms of information about the stress immediately implies that the former is inherently both constitutive and kinematic in nature. This contrasts with conventional ideas in continuum theory according to which kinematical and dynamical variables are viewed as being conceptually independent of a constitutive framework. The constitutive/geometric nature of the constituent elastic and plastic deformations affords considerable latitude in resolving ambiguities about their properties that are unavoidable in a purely geometric interpretation. The purpose if the present work is to extract definitive statements about these variables from specific constitutive hypotheses and thus to clarify the structure of initial-boundary-value problems for the motion of a continuum in the presence of plasticity. Our views combine three major lines of thought in the recent literature on plasticity. These are ($i$) the recognition of the constitutive character of elastic and plastic deformations [1], ($ii$) the central roles played by incompatibility and Eshelby's energy-momentum tensor [2,3], and (*iii*) the recognition of the primary role of dissipation in plastic evolution [4,5]. We concentrate on the purely mechanical theory as this is sufficient to highlight the issues of main concern.

The following notation is adopted in which $V$ is the translation (vector) space of a real three-dimensional Euclidean point space $E$:

$Lin$   the linear space of linear transformations (tensors) from $V$ to $V$.

$InvLin$   the group of invertible tensors.

$Sym = \{\mathbf{A} \in Lin\colon\ \mathbf{A} = \mathbf{A}^t$, the transpose of $\mathbf{A}\}$, the linear space of symmetric tensors; also, the linear operation of symmetrization on $Lin$.

$Skw = \{\mathbf{A} \in Lin\colon\ \mathbf{A}^t = -\mathbf{A}\}$, the linear space of skew tensors; also, the linear operation of skew-symmetrization on $Lin$.

$Orth^+ = \{\mathbf{A} \in InvLin\colon\ \mathbf{A}^t = \mathbf{A}^{-1}$, the inverse of $\mathbf{A}$, with $J_A = 1\}$, the group of rotations.

The determinant and cofactor of $\mathbf{A}$ are denoted by $J_A$ and $\mathbf{A}^*$, respectively, and $\mathbf{A}^* = J_A\mathbf{A}^{-t}$ if $\mathbf{A} \in InvLin$. It follows easily that $(\mathbf{AB})^* = \mathbf{A}^*\mathbf{B}^*$. Further, $Lin$ is equipped with the Euclidean inner product and norm defined by $\mathbf{A}\cdot\mathbf{B} = tr(\mathbf{AB}^t)$ and $|\mathbf{A}|^2 = \mathbf{A}\cdot\mathbf{A}$, respectively, where $tr(\cdot)$ is the trace. We make frequent use of relations like $\mathbf{A}\cdot\mathbf{BC} = \mathbf{AC}^t\cdot\mathbf{B} = \mathbf{C}^t\cdot\mathbf{A}^t\mathbf{B}$ and $\mathbf{AB}\cdot\mathbf{CD} = \mathbf{ABD}^t\cdot\mathbf{C}$, etc., which follow easily from $tr\mathbf{A} = tr(\mathbf{A}^t)$ and $tr(\mathbf{AB}) = tr(\mathbf{BA})$. It is well known that $Lin = Sym \oplus Skw$, the direct sum of $Sym$ and $Skw$, where $2Sym\mathbf{A} = \mathbf{A} + \mathbf{A}^t$ and $2Skw\mathbf{A} = \mathbf{A} - \mathbf{A}^t$. The tensor product $\mathbf{a}\otimes\mathbf{b}$ of vectors is defined by $(\mathbf{a}\otimes\mathbf{b})\mathbf{v} = (\mathbf{b}\cdot\mathbf{v})\mathbf{a}$ for all $\mathbf{v}$ in $V$, where $\mathbf{b}\cdot\mathbf{v}$ is the standard inner product of vectors. The gradient of a differentiable function $G\colon\ Lin \to \mathbb{R}$ is the tensor $G_{\mathbf{A}}$ defined by

$$G(\mathbf{A}+\mathbf{B}) = G(\mathbf{A}) + G_{\mathbf{A}}\cdot\mathbf{B} + o(|\mathbf{B}|). \tag{1}$$

A similar formula applies to differentiable vector-valued functions defined on $E$. Following standard practice we reserve the notation $\nabla$ for the associated gradient.

We assume the conventional balances of linear momentum and moment of momentum to apply to arbitrary parts of the body $B$. Thus,

$$div\mathbf{T} + \rho_t\mathbf{b} = \rho_t\mathbf{a}, \quad \mathbf{T} \in Sym \tag{2}$$

at points in the configuration $\kappa_t$ occupied by the body at time $t$, where $\mathbf{x}$ is the position therein of a material point $p \in B$, $\rho_t(\mathbf{x}, t)$ is the associated mass density, $div$ is the divergence operator based on $\mathbf{x}$, $\mathbf{a}$ is the material acceleration and $\mathbf{T}(\mathbf{x}, t)$ is the Cauchy stress. In practice the referential form

$$Div\mathbf{P} + \rho_r\mathbf{b} = \rho_r\ddot{\mathbf{x}}, \quad \text{where} \quad \mathbf{P} = \mathbf{TF}^* \tag{3}$$

is the Piola stress, is often most useful, where $Div$ is the divergence with respect to $\mathbf{X}$, the position of $p$ in a fixed reference placement $\kappa_r$ with mass density $\rho_r(\mathbf{X})$, superposed dots stand for material time derivatives ($\partial/\partial t$ at fixed $\mathbf{X}$), and where $\mathbf{F} = \nabla\boldsymbol{\chi}(\mathbf{X}, t)$ is the gradient at $p$ of the map $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$ from $\kappa_r$ to $\kappa_t$. We also assume the mass to be conserved, this being expressed simply by $\rho_r = \rho_t J_F$, where $J_F(>0)$ is the local ratio of volume in $\kappa_t$ to that in $\kappa_r$.

We are interested in applications of the theory to shock physics and thus append the jump relations [6]

$$U[\rho_r] = 0, \quad [\mathbf{P}]\mathbf{N} + U^2\rho_r[\dot{\mathbf{x}}] = \mathbf{0}, \tag{4}$$

where $\mathbf{N}$ is the local unit normal to a surface $S$ of discontinuity in $\kappa_r$ with speed $U$ in the direction of $\mathbf{N}$, and $[\cdot]$ is the discontinuity on $S$.

The basis of the idea of a local stress-free state, and an associated manifold of *intermediate* configurations, is examined in Section 2. This is grounded in the notion of an equilibrium unloading process together with appropriate constitutive hypotheses on the elastic response. In Section 3 the constituent elastic and plastic deformations are discussed. Stokes' theorem is used to describe the notion of incompatibility and associated dislocation densities. This is adapted, in Section 4, to describe surface dislocation in terms of discontinuous elastic and plastic deformation fields. Surface dislocation contributes to the net Burgers vector associated with a surface that intersects the discontinuity surface, and furnishes the extension of Hadamard's lemma for coherent interfaces to the non-coherent case. The extension effectively removes the severe rank-one constraint on the discontinuity imposed at a coherent interface, and thereby confers an additional degree of freedom on the kinematics of deformation. The basic constitutive framework is discussed in Section 5, where the elasticity of the body is described and the dissipation associated with plastic evolution is expressed in terms of Eshelby's tensor. Of central importance is the assumption introduced there of strong dissipation, according to which plastic evolution is inherently dissipative. This imposes a constraint on the kinds of evolution that qualify as plasticity, constituting, in effect, part of the definition of plastic flow. It is used, in Section 6, to derive unambiguous transformation rules for the elastic and plastic deformations under superposed rigid-body motions. Material symmetry restrictions on the elastic response and on constitutive equations for yield and plastic flow are discussed in Sections 7 and 8, following ideas put forth in [1] and [7]. Finally, in Section 8, the latitude afforded by the constitutive character of the plastic deformation is used to dispose of a long-standing controversy surrounding plastic spin.

## 2. Unloading elastic bodies to zero stress

A central tenet of the considered model is the idea that stress is purely elastic in origin, the associated deformation being measured from a stress-free local configuration. It is therefore of no small importance to have some justification of this assumption. To explore this issue we appeal to the mean-stress theorem, according to which the mean Cauchy stress in a body $B$ is zero if it is in equilibrium and subjected to vanishing surface tractions and body forces [8]. Thus, the mean stress

$$\bar{\mathbf{T}}(t) = [vol(\kappa_t)]^{-1}\int_{\kappa_t}\mathbf{T}(\mathbf{x},t)dV \tag{5}$$

vanishes, where $\mathbf{T}$ is the Cauchy stress and $vol(\kappa_t)$ is the volume of $\kappa_t$. This theorem is valid for stress fields that are differentiable and hence continuous in $\kappa_t$. The mean-value theorem is then applicable and guarantees the existence of $\bar{\mathbf{x}} \in \kappa_t$ such that $\mathbf{T}(\bar{\mathbf{x}},t) = \bar{\mathbf{T}}(= \mathbf{0})$. Let

$$d(\kappa_t) = \sup_{\mathbf{x},\mathbf{y}\in\kappa_t}|\mathbf{x}-\mathbf{y}| \tag{6}$$

be the diameter of $\kappa_t$. For $d \to 0$ we have $|\mathbf{x} - \bar{\mathbf{x}}| \to 0$ for all $\mathbf{x}$ in $\kappa_t$ and the continuity of $\mathbf{T}(\mathbf{x}, t)$ furnishes $\mathbf{T}(\mathbf{x}, t) \to \mathbf{T}(\bar{\mathbf{x}}, t) = \mathbf{0}$. Thus, if the hypotheses of the mean-stress theorem are satisfied, then the local stress can be brought arbitrarily close to zero by making the diameter of the body correspondingly small against any length scale at hand. This result is of course independent of material constitution and furnishes theoretical justification for the measurement of residual stress by cutting out a small part of a body and observing its change in shape.

For elastic bodies the Cauchy stress is given in terms of the deformation from a reference configuration $\kappa_r$ of $B$ by the well-known formula [9]

$$J_F \mathbf{T} = W_{\mathbf{F}} \mathbf{F}^t, \tag{7}$$

where $W(\mathbf{F})$ is the strain energy per unit volume of $\kappa_r$. The function $W(\mathbf{F})$ is frame invariant, in the sense that $W(\mathbf{F}) = W(\mathbf{QF})$ for any rotation $\mathbf{Q}$, if and only if it is determined by the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^t\mathbf{F}$; thus, $W(\mathbf{F}) = \hat{W}(\mathbf{C})$ and the well-known relation $W_{\mathbf{F}} = 2\mathbf{F}(Sym\hat{W}_{\mathbf{C}})$ furnishes

$$J_F \mathbf{T} = 2\mathbf{F}(Sym\hat{W}_{\mathbf{C}})\mathbf{F}^t. \tag{8}$$

The Cauchy stress vanishes if and only if $\hat{W}$ is stationary. Let $\kappa_r$ be stress free, so that $\hat{W}$ is stationary at $\mathbf{C} = \mathbf{I}$. We assume that $\mathbf{C} = \mathbf{I}$ is the unique stationary point. This is assured by adopting the constitutive assumption that the strain energy is a strictly convex function of $\mathbf{C}$ with a minimum at $\mathbf{C} = \mathbf{I}$. Thus, we assume that

$$\hat{W}(\mathbf{C}_2) - \hat{W}(\mathbf{C}_1) > Sym\hat{W}_{\mathbf{C}}(\mathbf{C}_1) \cdot (\mathbf{C}_2 - \mathbf{C}_1); \quad \mathbf{C}_2 \neq \mathbf{C}_1, \quad \text{with} \quad \hat{W}(\mathbf{I}) = 0 \quad \text{and} \quad Sym\hat{W}_{\mathbf{C}}(\mathbf{I}) = \mathbf{0}. \tag{9}$$

This in turn guarantees that stress relaxation is energetically optimal and reflects the phenomenology typical of metals in the elastic range provided that

$$|\mathbf{C} - \mathbf{I}| < \epsilon, \tag{10}$$

where $\epsilon$ depends on the material at hand.

To elaborate, imagine cutting $\kappa_t$ into an arbitrarily large number of sub-bodies of arbitrarily small diameter and relaxing the loads thereon. The mean-stress theorem together with our constitutive hypotheses imply that *equilibrium* states of these sub-bodies are stress-free, minimum-energy configurations in a Euclidean point space $E$ provided, as we assume here, that no energy is needed to generate the new surfaces created by this process. If these relaxed configurations cannot be made congruent in the absence of strain, then they do not fit together to form a connected whole in Euclidean space. The material is said to be *dislocated.* For a given sub-body, consider two relaxed configurations $\kappa_{r_1}$ and $\kappa_{r_2}$ in $E$ related by the map $\mathbf{X}_2 = \boldsymbol{\mu}(\mathbf{X}_1)$. Then $d\mathbf{X}_2 = \mathbf{A}d\mathbf{X}_1$ where $\mathbf{A}$, with $J_A > 0$, is the gradient of $\boldsymbol{\mu}$. Let $\mathbf{F}_1$ and $\mathbf{F}_2$, respectively, be the gradients of the maps of these configurations to $\kappa_t$ at the material point $p$. Thus, $d\mathbf{x} = \mathbf{F}_1 d\mathbf{X}_1 = \mathbf{F}_2 d\mathbf{X}_2 = \mathbf{F}_2\mathbf{A}d\mathbf{X}_1$, and therefore

$$\mathbf{F}_1 = \mathbf{F}_2\mathbf{A}. \tag{11}$$

We wish to characterize any non-uniqueness in the local unloading process and so require that $\mathbf{F}_1$ and

$\mathbf{F}_2$ generate the same Cauchy stress in $\kappa_t$:

$$(W_1)_{\mathbf{F}_1}(\mathbf{F}_1^*)^{-1} = \mathbf{T} = (W_2)_{\mathbf{F}_2}(\mathbf{F}_2^*)^{-1}, \tag{12}$$

where $W_1(\mathbf{F}_1)$ and $W_2(\mathbf{F}_2)$, respectively, are the strain-energy functions based on $\kappa_{r_1}$ and $\kappa_{r_2}$. These are related, modulo a constant, by

$$W_1(\mathbf{F}_1) = J_A W_2(\mathbf{F}_2). \tag{13}$$

To see this consider a parametrized path of deformations and let a superposed dot denote the derivative with respect to the parameter. Using $\dot{W} = W_{\mathbf{F}} \cdot \dot{\mathbf{F}} = \mathbf{T}\mathbf{F}^* \cdot \dot{\mathbf{F}}$ with $\mathbf{A}$ fixed, we then obtain

$$\dot{W}_1(\mathbf{F}_1) = \mathbf{T}\mathbf{F}_1^* \cdot \dot{\mathbf{F}}_1 = \mathbf{T}\mathbf{F}_2^*\mathbf{A}^* \cdot \dot{\mathbf{F}}_2\mathbf{A} = \mathbf{T}\mathbf{F}_2^*\mathbf{A}^*\mathbf{A}^t \cdot \dot{\mathbf{F}}_2 = J_A \dot{W}_2(\mathbf{F}_2), \tag{14}$$

and hence (13).

The Cauchy stress vanishes at $p$ if and only if

$$Sym[(\hat{W}_1)_{\mathbf{C}_1}] = \mathbf{0} \quad \text{and} \quad Sym[(\hat{W}_2)_{\mathbf{C}_2}] = \mathbf{0}, \tag{15}$$

where

$$\hat{W}_1(\mathbf{C}_1) = J_A \hat{W}_2(\mathbf{C}_2) \quad \text{and} \quad \mathbf{C}_1 = \mathbf{A}^t\mathbf{C}_2\mathbf{A}. \tag{16}$$

Our constitutive hypotheses, applied to both strain-energy functions, then imply that $\mathbf{C}_1 = \mathbf{C}_2 = \mathbf{I}$ and hence that $\mathbf{A}^t\mathbf{A} = \mathbf{I}$. Thus,

$$\mathbf{A} \in Orth^+. \tag{17}$$

Since this holds identically in the given sub-body, the fact that $\mathbf{A}$ is the gradient of a map $\boldsymbol{\mu}$ implies that $\mathbf{A}$ is uniform [10; pp. 49, 50]. The unloading process then determines a local relaxed configuration in $E$ modulo orientation and translation. This degree of freedom is seen to follow directly from our constitutive hypotheses and the consequent interplay between deformation and stress in the definition of unloading.

We identify an arbitrarily small open ball surrounding a material point $p \in B$ with a tangent space to a global differentiable manifold $\mathcal{M}$. Let $\mathbf{F}$ map the tangent space $T_{\mathcal{M}(p)}$ of $\mathcal{M}$ at $p$ to $V$ at $\mathbf{x}$ in $\kappa_t$. We stipulate that $\mathbf{F}^t\mathbf{F}$ be the strain at $p$ required to make the collection of stress-free sub-bodies in $E$ fit together in $\kappa_t$. The non-existence of a global differentiable map from $\kappa_t$ to the disjoint relaxed sub-bodies in $E$ implies that points $p$ in the unstressed manifold $\mathcal{M}$ cannot be associated with a position field and thus that $\mathcal{M}$ is not Euclidean. The field $\mathbf{F}$ does not then satisfy the usual compatibility condition which follows from the existence of such a map. The incompatibility is typically identified with a distribution of Burgers vectors via an analogy with the geometry of defective crystal lattices. This idea is the basis of the elegant differential-geometric theory of self-stressed bodies containing continuously distributed dislocations [11-19].

Our assumption of a unique energy well in the domain of $\hat{W}$ excludes certain models of crystal elasticity proposed by Ericksen [20] and Hill [21]. These models are motivated by the observation that there exist unimodular non-orthogonal transformations of a regular cubic lattice, say, which generate lattices that are geometric copies of each other. If $W_1(\mathbf{F})$ and $W_2(\mathbf{F})$ are the strain-energy functions for two lattices related in this manner, then it is natural to assume that they respond identically to a given deformation and thus that they satisfy the symmetry condition

$$W_1(\mathbf{F}) = W_2(\mathbf{F}). \tag{18}$$

Our view (see also [22]) is that symmetries of this kind do not fit naturally in the framework of Noll's simple elastic solid [23]. For, if $\mathbf{G}$ is an element of the symmetry set of the first lattice, then by Noll's Rule $\mathbf{KGK}^{-1}$ belongs to the symmetry set of the second, where $\mathbf{K}$ is the gradient of the deformation that carries the first lattice to the second. We then have

$$W_1(\mathbf{F}) = W_1(\mathbf{FG}) \quad \text{and} \quad W_2(\mathbf{F}) = W_2(\mathbf{FKGK}^{-1}), \tag{19}$$

which imply that $\mathbf{G} = \mathbf{K}$ and $\mathbf{G} = \mathbf{K}^{-1}$ are symmetry transformations for both (hence all) lattices so related. Thus,

$$W(\mathbf{F}) = W(\mathbf{FK}) = W(\mathbf{FK}^{-1}), \tag{20}$$

where $W$ stands for $W_1$ or $W_2$. Let $\mathbf{e}_i$; $i = 1, 2, 3$, be the axes of the first cubic lattice, normalized by the (uniform) lattice spacing and aligned with the edges of a typical cube. Then a transformation of the required type is furnished by the simple shear $\mathbf{K} = \mathbf{I} + \gamma\mathbf{e}_1 \otimes \mathbf{e}_2$, where $\gamma$ is an integral multiple (positive or negative) of the lattice spacing. The inverse of $\mathbf{K}$ is a simple shear of amount $-\gamma$ and also furnishes a map of the lattice to itself. The presence of such $\mathbf{K}$ and its inverse in the symmetry set is thus to be expected on physical grounds. In turn, this implies that $\mathbf{K}^t\mathbf{CK}$ belongs to the domain of the strain-energy function $\hat{W}$ whenever $\mathbf{C}$ does, for any amount of shear equal to an integral multiple (positive or negative) of the lattice spacing. Elastic response of this kind may be understood by regarding the bonds between atoms at the corners of a lattice cell as nonlinear springs. This analogy suggests that Noll's simple elastic material does not furnish an acceptable model of the physics at hand as arbitrarily large spring extensions would have to be admitted, whereas interatomic bonds presumably fail to persist when extended beyond finite limits.

Here, we discard the elastic interpretation and instead adopt the mechanism of plasticity to account for the underlying phenomenon. Thus, we re-interpret (18) as a statement to the effect that the *elastic* response of the lattice to a deformation $\mathbf{F}$ is unaffected by *plastic* slip $\mathbf{K}$ (or $\mathbf{K}^{-1}$). We retain Noll's view insofar as a superposed elastic distortion $\mathbf{F}$ is concerned. Variations in $\mathbf{F}$ at fixed $\mathbf{K}$ generate variations in stress in accordance with the elastic properties of the crystal, provided that such variations engender non-zero strains belonging to the domain of the elastic constitutive function. Thus, we introduce an elastic energy and confine symmetry transformations to subgroups of the orthogonal group, in accordance with Noll's original distinction between simple solids and simple fluids [23]. Such transformations preserve inequality (10) and the energy-minimizing value, $\mathbf{I}$, of $\mathbf{C}$. To model the invariance embodied in (18), it is then necessary to extend the constitutive structure beyond Noll's simple elastic solid to encompass the evolution of $\mathbf{K}$. This of course is precisely the aim of Plasticity Theory. The shortcomings of Noll's simple materials as models of plasticity are discussed further in [4, 24].

The connection between (20) and plasticity seems to be what Ball and James [25] have in mind in their discussion of lattice symmetry. Specifically, their view is that the domain of the strain-energy function should be limited in accordance with a restriction like (10) above so as to exclude from the symmetry group of the elastic response function the possibly large lattice shears typically associated with plasticity. The adjustment means that if $\mathbf{C}$ belongs to the domain of $\hat{W}$ then $\mathbf{K}^t\mathbf{C}\mathbf{K}$ does not, if the amount of shear is sufficiently large. Instead, the latter would necessarily be associated with inelastic behavior. The restriction advocated by Ball and James excludes such shears from the theory of the elastic response of crystals. To effect such exclusion it is sufficient to assume (10) and to restrict the symmetry set to a subset of the orthogonal group.

### 3. Deformation and incompatibility

The foregoing considerations lead us to introduce a local stress-free *intermediate* configuration $\kappa_i$ of a material point $p$ and to identify this with the tangent space $T_{\mathcal{M}(p)}$ at $p$ to a differentiable manifold $\mathcal{M}$ having a generally non-Euclidean structure. The properties of this manifold may be inferred from our discussion but are not needed explicitly in this work. We reserve the labels $\kappa_r$ and $\kappa_t$ for global reference and current configurations of $B$, respectively. These are regions in the Euclidean point space $E$. The positions of a point $p \in B$ in $\kappa_r$ and $\kappa_t$ are denoted by $\mathbf{X}$ and $\mathbf{x}$, respectively, and we assume the existence of an invertible differentiable map $\boldsymbol{\chi}_{\kappa_r}$ such that $\mathbf{x} = \boldsymbol{\chi}_{\kappa_r}(\mathbf{X}, t)$. The subscript is suppressed unless it is needed for clarity and we typically write $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$. Let $\mathbf{F}$ be the gradient of the deformation from $\kappa_r$ to $\kappa_t$:

$$\mathbf{F} = \nabla\boldsymbol{\chi}(\mathbf{X}, t), \tag{21}$$

where $\nabla$ is the gradient with respect to $\mathbf{X}$. Let $\mathbf{H}$ be the local map from the tangent space $\kappa_i$ to $V$ at $\mathbf{x} \in \kappa_t$, and let $\mathbf{K}$ be the map from $\kappa_i$ to $V$ at $\mathbf{X} \in \kappa_r$. We assume that $J_H$ and $J_K$ are positive. Thus, $\mathbf{H}$ and $\mathbf{K}^{-1}$ are the *elastic* and *plastic* deformations, respectively. Unlike $\mathbf{F}$, they are not, in general, gradients of position fields. This issue is associated with the fact that position fields do not exist in $\mathcal{M}$ due to its non-Euclidean character. We have [2]

$$\mathbf{H} = \mathbf{F}\mathbf{K}. \tag{22}$$

An adaptation of Stokes' theorem [14, 26, 27] furnishes

$$\int_{\partial S} \mathbf{F}d\mathbf{X} = \int_S (Curl\mathbf{F})^t\mathbf{N}dA, \tag{23}$$

where $S$, with boundary $\partial S$, is an oriented surface in a simply-connected region of $\kappa_r$ with local unit-normal field $\mathbf{N}(\mathbf{X})$ for $\mathbf{X} \in S$, and $Curl$ is the referential curl operator. This theorem holds if $\mathbf{F}$ is a differentiable function of $\mathbf{X}$. The curl is defined in terms of the usual curl operation on vector fields by [26, 27]

$$(Curl\mathbf{A})\mathbf{c} = Curl(\mathbf{A}^t\mathbf{c}); \quad \mathbf{c} \quad \text{fixed}, \tag{24}$$

which furnishes (23) as an immediate consequence of Stokes' theorem for vector fields. From (21) we have that $\mathbf{F}d\mathbf{X} = d\boldsymbol{\chi}$ and the left-hand side of (23) vanishes. The arbitrariness of $S$ and thus of its local orientation $\mathbf{N}$ then implies that $Curl\mathbf{F} = \mathbf{0}$ in $\kappa_r$. This also follows directly from the differentiability of $\nabla\boldsymbol{\chi}$. Conversely, if $Curl\mathbf{F} = \mathbf{0}$ in a simply-connected part of $\kappa_r$ containing $S$ then the right-hand side of (23) vanishes. This implies that the line integral $\int_\Gamma \mathbf{F}d\mathbf{X}$ is independent of the path $\Gamma$ in such a region and thus, following a classical argument [28; Sect. 59], that $\mathbf{F}$ is the gradient of a (vector) potential which we identify with the deformation $\boldsymbol{\chi}$. It follows that the vanishing of $Curl\mathbf{F}$ is necessary and sufficient for *compatibility* of $\mathbf{F}$ in a simply-connected region; i.e., for the existence of a position field $\boldsymbol{\chi}(\mathbf{X}, t)$ such that $\nabla\boldsymbol{\chi} = \mathbf{F}$.

The properties of the manifold $\mathcal{M}$ imply that $Curl\mathbf{K}^{-1}$ need not vanish. In this case we define

$$\mathbf{B}(S,t) \doteq \int_{\partial S} \mathbf{K}^{-1} d\mathbf{X} = \int_S (Curl\mathbf{K}^{-1})^t \mathbf{N} dA, \tag{25}$$

where the right-most equality follows if the field $\mathbf{K}^{-1}$ is smooth. This is referred to as the Burgers vector associated with $S$ in recognition of its interpretation in dislocation theory. Thus, the existence of a non-zero Burgers vector is due to the incompatibility of the plastic deformation or, equivalently, to the non-existence of a position field in $\mathcal{M}$ with (referential) gradient $\mathbf{K}^{-1}$. Using the (smooth) elastic deformation instead, we define

$$\mathbf{b}(s,t) \doteq \int_{\partial s} \mathbf{H}^{-1} d\mathbf{x} = \int_s (curl\mathbf{H}^{-1})^t \mathbf{n} da, \tag{26}$$

where $s$ is the image in $\kappa_t$ of $S \subset \kappa_r$ with unit-normal field $\mathbf{n}(\mathbf{x}, t)$ and *curl* is the spatial curl operator based on $\mathbf{x}$. It follows from (22) and Nanson's formula $\mathbf{n}da = \mathbf{F}^*\mathbf{N}dA$ that $\mathbf{b}(s,t) = \mathbf{B}(S,t)$ [26]. Then $\mathbf{H}^{-1}(\mathbf{x}, t)$ is incompatible if and only if $\mathbf{K}^{-1}(\mathbf{X}, t)$ is incompatible. The tensors

$$\boldsymbol{\alpha}_r = Curl\mathbf{K}^{-1} \quad \text{and} \quad \boldsymbol{\alpha}_t = curl\mathbf{H}^{-1} \tag{27}$$

thus provide measures of the incompatibility per unit area of a material surface in $\kappa_r$ and $\kappa_t$, respectively. Accordingly, we refer to these as the referential and spatial dislocation densities.

In [26] an associated tensor $\boldsymbol{\alpha}$ called the *true dislocation density* is introduced. This satisfies

$$J_K \mathbf{K}^{-1} Curl\mathbf{K}^{-1} = \boldsymbol{\alpha} = J_H \mathbf{H}^{-1} curl\mathbf{H}^{-1}, \tag{28}$$

wherein the outer equality may be shown to follow from (22). The name is justified by the remarkable fact that $\boldsymbol{\alpha}$ is invariant under arbitrary differentiable variations of the configurations $\kappa_r$ and $\kappa_t$. To see this we consider a variation of $\kappa_r$ from $\kappa_{r_1}$ to $\kappa_{r_2}$ defined by the one-to-one map $\mathbf{X}_2 = \boldsymbol{\lambda}(\mathbf{X}_1)$ with invertible gradient $\mathbf{R} = \nabla_1\boldsymbol{\lambda}$, where $\nabla_1$ is the gradient with respect to $\mathbf{X}_1$. Using obvious notation we have $\mathbf{K}_1^{-1} d\mathbf{X}_1 = \mathbf{K}_2^{-1} d\mathbf{X}_2$ and therefore

$$\int_{S_2} (Curl_2\mathbf{K}_2^{-1})^t \mathbf{N}_2 dA_2 = \int_{\partial S_2} \mathbf{K}_2^{-1} d\mathbf{X}_2 = \int_{\partial S_1} \mathbf{K}_1^{-1} d\mathbf{X}_1 = \int_{S_1} (Curl_1\mathbf{K}_1^{-1})^t \mathbf{N}_1 dA_1, \tag{29}$$

where $S_2 = \lambda(S_1)$, provided that

$$\mathbf{K}_2 = \mathbf{R}\mathbf{K}_1. \tag{30}$$

Nanson's formula in the form $\mathbf{N}_2 dA_2 = \mathbf{R}^*\mathbf{N}_1 dA_1$ and the arbitrariness of $S_1$ then combine to give [26]

$$J_R Curl_2 \mathbf{K}_2^{-1} = \mathbf{R} Curl_1 \mathbf{K}_1^{-1}, \tag{31}$$

which yields the invariance of $\boldsymbol{\alpha}$ by virtue of $(28)_1$ and $J_{K_1} J_R = J_{K_2}$. Further, (30) and (31) may be used with an obvious adjustment in notation to establish the outer equation in (28) directly. The same reasoning based on the second of eqs. (28) proves the invariance of $\boldsymbol{\alpha}$ under arbitrary one-to-one differentiable variations of $\kappa_t$. In effect $\boldsymbol{\alpha}$ furnishes a measure of dislocation in the body *per se* in the sense that it is insensitive to the placement of the body in any configuration in $E$. It is thus no coincidence that $\boldsymbol{\alpha}$ is associated with an intrinsic property of the material manifold $\mathcal{M}$, namely the *torsion* of the affine connection induced by $\mathbf{K}^{-1}$ and its (referential) gradient (or $\mathbf{H}^{-1}$ and its spatial gradient) [15, 16].

## 4. Interfaces

We have seen that if $\mathbf{K}^{-1}$ is a smooth function of $\mathbf{X}$ in a simply connected region of $\kappa_r$, then there exists a dislocation density $\boldsymbol{\alpha}_r$ defined on $\kappa_r$ such that

$$\mathbf{B}(S_\perp, t) = \int_{S_\perp} \boldsymbol{\alpha}_r^t \mathbf{N}_\perp dA, \tag{32}$$

where $\boldsymbol{\alpha}_r = Curl\mathbf{K}^{-1}$ and $S_\perp$ is any orientable open surface in said region with local orientation field $\mathbf{N}_\perp$. If $\boldsymbol{\alpha}_r$ does not vanish identically then the body is dislocated in this region. Consider a surface $S \subset \kappa_r$ of discontinuity of the plastic deformation $\mathbf{K}^{-1}$ and suppose $S_\perp$ cuts $S$ orthogonally. Let $\Gamma = S \cap S_\perp$ be the curve of intersection. If $\mathbf{K}^{-1}$ is differentiable in the regions on either side of $S$, then Stokes' theorem, and hence (32), may be applied to the individual parts $S_\perp^\pm$ of $S_\perp$ separated by $S$. Adding the two expressions and using $\Gamma = \partial S_\perp^+ \cap \partial S_\perp^-$, we then have

$$\int_{S_\perp} \boldsymbol{\alpha}_r^t \mathbf{N}_\perp dA = \int_{S_\perp^+ \cup S_\perp^-} (Curl\mathbf{K}^{-1})^t \mathbf{N}_\perp dA = \int_{\partial S_\perp} \mathbf{K}^{-1} d\mathbf{X} + \int_\Gamma [\mathbf{K}^{-1}] d\mathbf{X}, \tag{33}$$

where $[\mathbf{K}^{-1}] = (\mathbf{K}^{-1})^+ - (\mathbf{K}^{-1})^-$. We use the superscripts $^\pm$ to denote the limits of functions defined on $\kappa_r$ as $S$ is approached from the regions into which $\mathbf{N}$ and $-\mathbf{N}$ are directed, respectively, where $\mathbf{N}$ is the unit-normal field on $S$. We also use square brackets, as indicated, to denote the ordered difference between these limits. Let $\mathbf{t} = \mathbf{N}_\perp \mid_\Gamma$, so that $d\mathbf{X} = \mathbf{N} \times \mathbf{t} du$ in the final integral, where $u$ measures arclength on $\Gamma$. We define a tensor field $\boldsymbol{\beta}_r$ on $S$ - the (referential) *surface dislocation density* - such that

$$[\mathbf{K}^{-1}](\mathbf{t} \times \mathbf{N}) = \boldsymbol{\beta}_r^t \mathbf{t} \quad \text{on } S, \text{ for all unit } \mathbf{t} \in T_{S(\mathbf{X})}, \tag{34}$$

the tangent plane to $S$ at $\mathbf{X}$. The net Burgers vector associated with $S_\perp$ is then given by

$$\mathbf{B}(S_\perp, t) = \int_{S_\perp} \boldsymbol{\alpha}_r^t \mathbf{N}_\perp dA + \int_\Gamma \boldsymbol{\beta}_r^t \mathbf{t} du. \tag{35}$$

Let $\mathbf{t}_1, \mathbf{t}_2 \in T_{S(\mathbf{X})}$ be such that $\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{N}\}$ is a positively-oriented orthonormal basis. Writing $[\mathbf{K}^{-1}] = [\mathbf{K}^{-1}]\mathbf{I}$ with $\mathbf{I} = \mathbf{N} \otimes \mathbf{N} + \mathbf{t}_\alpha \otimes \mathbf{t}_\alpha$ leads to

$$[\mathbf{K}^{-1}] = \mathbf{k} \otimes \mathbf{N} - \boldsymbol{\beta}_r^t \boldsymbol{\varepsilon}_{(\mathbf{N})}, \tag{36}$$

where $\mathbf{k}$ is an arbitrary 3-vector and

$$\boldsymbol{\varepsilon}_{(\mathbf{N})} = \mathbf{t}_1 \otimes \mathbf{t}_2 - \mathbf{t}_2 \otimes \mathbf{t}_1 \tag{37}$$

is the two-dimensional permutation tensor density on $T_{S(\mathbf{X})}$. This satisfies $\boldsymbol{\varepsilon}_{(\mathbf{N})} = \mathbf{R}\boldsymbol{\varepsilon}_{(\mathbf{N})}\mathbf{R}^t$ for all two-dimensional orthogonal transformations $\mathbf{R}$ that preserve the orientation of $T_{S(\mathbf{X})}$. Therefore any pair of vectors in $T_{S(\mathbf{X})}$ which with $\mathbf{N}$ form a positive orthonormal basis may be used in the definition of $\boldsymbol{\varepsilon}_{(\mathbf{N})}$.

We may solve (36) using $\boldsymbol{\varepsilon}^2_{(\mathbf{N})} = -\mathbf{1}_{(\mathbf{N})}$, where $\mathbf{1}_{(\mathbf{N})} = \mathbf{I} - \mathbf{N}\otimes\mathbf{N}$ is the identity for $T_{S(\mathbf{X})}$, to obtain

$$\boldsymbol{\beta}^t_r \mathbf{1}_{(\mathbf{N})} = [\mathbf{K}^{-1}]\boldsymbol{\varepsilon}_{(\mathbf{N})}. \tag{38}$$

This determines the action of $\boldsymbol{\beta}^t_r$ on $T_{S(\mathbf{X})}$. The action of $\boldsymbol{\beta}^t_r$ on $\mathbf{N}$ is indeterminate and may be set to zero without loss of generality. The formula (38) is equivalent to a result stated by Bilby [29] and used extensively in the subsequent literature on crystal interfaces and grain boundaries [30, 31]. Bilby's result is not consistent with his definition of surface dislocation density as stated in the text of [29]. He defines the latter to be the finite limit obtained by invoking Stokes' theorem, collapsing $S_\perp$ onto $\Gamma$, and requiring the dislocation density $\boldsymbol{\alpha}_r$ to become unbounded. However, the indicated limit vanishes under conditions in which Stokes' theorem is valid. More recently, surface dislocation density has been defined in terms of discontinuities of crystal lattice vectors across $S$ using a formula equivalent to (33) [32].

If $\mathbf{K}^{-1}$ is the gradient of a continuous and piecewise twice differentiable deformation, then the second and third integrals in (33) vanish. The arbitrariness of $\Gamma$ then implies that $[\mathbf{K}^{-1}](\mathbf{t}\times\mathbf{N}) = \mathbf{0}$ for all $\mathbf{t}\in T_{S(\mathbf{X})}$, yielding Hadamard's formula $[\mathbf{K}^{-1}] = \mathbf{k}\otimes\mathbf{N}$ for a coherent interface [33]. Equations (36) and (38) extend Hadamard's result to general non-coherent (i.e., dislocated) interfaces.

Proceeding from (26) and $(27)_2$ instead, we derive

$$[\mathbf{H}^{-1}] = \mathbf{h}\otimes\mathbf{n} - \boldsymbol{\beta}^t_t\boldsymbol{\varepsilon}_{(\mathbf{n})} \quad \text{and} \quad \boldsymbol{\beta}^t_t\mathbf{1}_{(\mathbf{n})} = [\mathbf{H}^{-1}]\boldsymbol{\varepsilon}_{(\mathbf{n})}, \tag{39}$$

where $\mathbf{h}$ is an arbitrary 3-vector, $\mathbf{n}$ is the orientation of a surface $s\subset\kappa_t$ of discontinuity of $\mathbf{H}^{-1}(\mathbf{x},t)$ and $\boldsymbol{\beta}_t$ is the spatial surface dislocation density. This emerges from an obvious adjustment to (33), and reduces in the coherent case to Hadamard's rank-one form $[\mathbf{H}^{-1}] = \mathbf{h}\otimes\mathbf{n}$. Evidently the generalization to non-coherent interfaces yields a full-rank expression which relaxes the constraint on the limits $(\mathbf{H}^{-1})^\pm$ associated with a coherent interface. Accordingly, surface dislocation is an additional interfacial degree of freedom which is available to minimize the elastic energy in the adjoining material. In general, this implies that non-coherent interfaces are energetically optimal, which presumably accounts for the stress relaxation typically attributed to the mechanism of surface dislocation. For example, our constitutive hypotheses imply that adjoining crystal grains are in their minimum-energy states if $\mathbf{H}^t\mathbf{H} = \mathbf{I}$ therein. By the polar decomposition theorem, $\mathbf{H}^{-1}$ then reduces to a rotation in each grain, and $(39)_2$ furnishes the required surface dislocation density in terms of the rotation discontinuity. The so-called *tilt* and *twist* boundaries furnish illustrative examples [14; Sec. 3.9].

The referential and spatial surface dislocation densities are not independent. For, if $s$ is the image of $S$ under the overall deformation, i.e. if $s = \chi(S,t)$, then the existence of a continuous inverse deformation $\boldsymbol{\chi}^{-1}(\mathbf{x},t)$ mapping $\kappa_t$ to $\kappa_r$ implies that any jump in $\mathbf{F}^{-1}$ is of Hadamard's form $[\mathbf{F}^{-1}] = \mathbf{a}\otimes\mathbf{n}$. Using this in the inverse of (22) together with

$$[\mathbf{H}^{-1}] = \left\langle\mathbf{K}^{-1}\right\rangle[\mathbf{F}^{-1}] + [\mathbf{K}^{-1}]\left\langle\mathbf{F}^{-1}\right\rangle, \tag{40}$$

where $\langle\cdot\rangle$ is the average of the limits of the enclosed function on either side of the interface, we derive

$$\mathbf{h}\otimes\mathbf{n} - \boldsymbol{\beta}^t_t\boldsymbol{\varepsilon}_{(\mathbf{n})} = \left\langle\mathbf{K}^{-1}\right\rangle\mathbf{a}\otimes\mathbf{n} + \mathbf{k}\otimes\left\langle\mathbf{F}^{-t}\right\rangle\mathbf{N} - \boldsymbol{\beta}^t_r\boldsymbol{\varepsilon}_{(\mathbf{N})}\left\langle\mathbf{F}^{-1}\right\rangle. \tag{41}$$

Nanson's formula ensures that $\langle \mathbf{F}^{-t} \rangle \mathbf{N}$ is parallel to $\mathbf{n}$. Multiplication on the right by $\boldsymbol{\varepsilon}_{(\mathbf{n})}$ thus furnishes $\boldsymbol{\beta}_t^t$ in terms of $\boldsymbol{\beta}_r^t$:

$$\boldsymbol{\beta}_t^t \mathbf{1}_{(\mathbf{n})} = -\boldsymbol{\beta}_r^t \boldsymbol{\varepsilon}_{(\mathbf{N})} \left\langle \mathbf{F}^{-1} \right\rangle \boldsymbol{\varepsilon}_{(\mathbf{n})}, \tag{42}$$

and the normal component of (41) yields a relationship among the vectors $\mathbf{a}, \mathbf{k}$ and $\mathbf{h}$:

$$\mathbf{h} = \left\langle \mathbf{K}^{-1} \right\rangle \mathbf{a} + (\mathbf{n} \cdot \left\langle \mathbf{F}^{-t} \right\rangle \mathbf{N})\mathbf{k} - \boldsymbol{\beta}_r^t \boldsymbol{\varepsilon}_{(\mathbf{N})} \left\langle \mathbf{F}^{-1} \right\rangle \mathbf{n}. \tag{43}$$

There is no requirement that $S \subset \kappa_r$ be a material surface. If it is not, then

$$U[\mathbf{F}] + [\dot{\mathbf{x}}] \otimes \mathbf{N} = \mathbf{0}, \tag{44}$$

provided that the deformation is continuous, where $U$ is the velocity of $S$ in the direction of $\mathbf{N}$ [6]. Using this with

$$[\mathbf{F}] \left\langle \mathbf{F}^{-1} \right\rangle + \langle \mathbf{F} \rangle [\mathbf{F}^{-1}] = \mathbf{0}, \tag{45}$$

we derive

$$[\dot{\mathbf{x}}] \otimes \left\langle \mathbf{F}^{-t} \right\rangle \mathbf{N} = U \langle \mathbf{F} \rangle \mathbf{a} \otimes \mathbf{n}. \tag{46}$$

## 5. Stored energy and dissipation

The elastic response is assumed to be described by a strain-energy function $W(\mathbf{H})$ per unit volume of a reference configuration. This function describes the response of the material to distortion induced by the map from $\kappa_i$ to $V$ at $\mathbf{x} \in \kappa_t$. Mainly for illustrative purposes, we confine attention here to functions $W(\mathbf{H})$ that do not vary from one material point to another. This restriction defines *materially uniform* bodies [7, 15, 16]. Let $\Psi$ be the strain energy per unit volume of $\kappa_r$. Then, from (22), $\Psi$ may be regarded as a function of $\mathbf{F}$ and $\mathbf{K}$ defined by

$$\Psi(\mathbf{F}, \mathbf{K}) = J_K^{-1} W(\mathbf{FK}). \tag{47}$$

The strain energy at fixed $\mathbf{K}$ is given by $\Psi_K(\mathbf{F}, \mathbf{X}) = \Psi(\mathbf{F}, \mathbf{K}(\mathbf{X}))$ and depends explicitly on $\mathbf{X}$ only if the distribution of plastic deformation is not uniform.

We assume the stress to be purely elastic in origin and thus impose (7) with $\mathbf{F}$ replaced by $\mathbf{H}$:

$$J_H \mathbf{T} = W_{\mathbf{H}} \mathbf{H}^t. \tag{48}$$

Using $\mathbf{P} = \mathbf{TF}^*$ with $\mathbf{F}^*\mathbf{K}^* = \mathbf{H}^*$, we then derive

$$W_{\mathbf{H}} = \mathbf{PK}^*. \tag{49}$$

This furnishes

$$\dot{W} = \mathbf{PK}^* \cdot \dot{\mathbf{H}} = J_K \mathbf{P} \cdot \dot{\mathbf{H}} \mathbf{K}^{-1}, \tag{50}$$

yielding

$$\mathbf{P} \cdot \dot{\mathbf{F}} = \dot{\Psi} \quad \text{if} \quad \dot{\mathbf{K}} = \mathbf{0}. \tag{51}$$

In the general case, we use

$$\dot{\Psi} = J_K{}^{-1}[\dot{W} - (\dot{J}_K/J_K)W] \tag{52}$$

with

$$\dot{J}_K/J_K = \mathbf{K}^{-t} \cdot \dot{\mathbf{K}}, \tag{53}$$

$$\dot{W} = W_{\mathbf{H}} \cdot \dot{\mathbf{H}} = W_{\mathbf{H}}\mathbf{K}^t \cdot \dot{\mathbf{F}} + \mathbf{F}^t W_{\mathbf{H}} \cdot \dot{\mathbf{K}}, \tag{54}$$

and (49), to obtain

$$\dot{\Psi} = \mathbf{P} \cdot \dot{\mathbf{F}} + J_K^{-1}(\mathbf{F}^t\mathbf{P} - W\mathbf{I})\mathbf{K}^* \cdot \dot{\mathbf{K}}, \tag{55}$$

which may be recast as

$$\mathbf{P} \cdot \dot{\mathbf{F}} = \dot{\Psi} + D, \tag{56}$$

where

$$D = \mathcal{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} \tag{57}$$

and where

$$\mathcal{E} = \Psi\mathbf{I} - \mathbf{F}^t\mathbf{P} \tag{58}$$

is Eshelby's energy-momentum tensor [34]. These results, due to Epstein and Maugin [2], have been reproduced in several forms in the subsequent literature [3, 5, 35-37].

Further, using (47) and (49), Eshelby's tensor may be written in the form

$$\mathcal{E} = J_K^{-1}\mathbf{K}^{-t}\mathcal{E}'\mathbf{K}^t, \tag{59}$$

where

$$\mathcal{E}' = W\mathbf{I} - \mathbf{H}^t W_{\mathbf{H}} \tag{60}$$

is purely elastic in origin. This in turn yields

$$J_K D = \mathcal{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}}. \tag{61}$$

Equation (56) furnishes a decomposition of the stress power per unit volume of $\kappa_r$ into an energetic part and a part arising from the evolution of plastic deformation. Following conventional ideas we assume the part not accounted for by the energy to be dissipated, i.e.

$$D \geq 0 \quad \text{for all} \quad \dot{\mathbf{K}}. \tag{62}$$

It is obvious that $D$ vanishes if $\dot{\mathbf{K}}$ vanishes. It is natural to expect that the converse is also true; i.e., that $D$ vanishes *only* if $\dot{\mathbf{K}}$ vanishes. This is tantamount to the assumption that the evolution of plasticity is *inherently dissipative*. In effect, this restriction *defines* plastic evolution in part through a constitutive assumption. Thus, we adopt the hypothesis:

$$\mathcal{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} > 0 \quad \text{if and only if} \quad \dot{\mathbf{K}} \neq \mathbf{0}. \tag{63}$$

A jump condition restricting the evolution of discontinuities may be obtained by specializing the Clausius-Duhem inequality. The relevant analysis is summarized in [6] and yields

$$U\mathbf{N} \cdot ([\mathcal{E}] + \tfrac{1}{2}\rho_r U^2[\mathbf{F}^t\mathbf{F}])\mathbf{N} \geq 0. \tag{64}$$

## 6. Superposed rigid motions

Granted the symmetry of the Cauchy stress, (48) implies that

$$W_{\mathbf{H}} \cdot \mathbf{\Omega H} = 0 \tag{65}$$

for any fixed $\mathbf{\Omega} \in Skw$. Consider a parametrized path $\mathbf{H}(u)$ defined by $\dot{\mathbf{H}}(u) = \mathbf{\Omega H}$ with $\mathbf{H}(0) = \mathbf{H}_0$. The unique solution [10] is $\mathbf{H}(u) = \mathbf{Q}(u)\mathbf{H}_0$, where $\mathbf{Q}$ is a rotation with $\mathbf{Q}(0) = \mathbf{I}$ and $\dot{\mathbf{Q}}\mathbf{Q}^t = \mathbf{\Omega}$. This means that $\dot{W} = 0$ on the path in question; i.e., that $W(\mathbf{QH}_0) = W(\mathbf{H}_0)$ for any rotation $\mathbf{Q}$. Standard arguments based on Cauchy's theorem for hemitropic functions [9] or on the polar decomposition theorem then furnish (with the subscript $_0$ suppressed)

$$W(\mathbf{H}) = \hat{W}(\mathbf{C}_H), \quad \text{where} \quad \mathbf{C}_H = \mathbf{H}^t\mathbf{H}, \tag{66}$$

and thus

$$J_H\mathbf{T} = \mathbf{HS}(\mathbf{C}_H)\mathbf{H}^t, \tag{67}$$

as in (8), where

$$\mathbf{S}(\mathbf{C}_H) = 2Sym\hat{W}_{\mathbf{C}_H}. \tag{68}$$

Henceforth we assume that all constitutive hypotheses introduced in Section 2 apply to the function $\hat{W}(\mathbf{C}_H)$.

Note that in the course of deriving (67) we have assumed only the symmetry of the Cauchy stress. In particular, we have not imposed the invariance of the strain-energy function under superposed rigid-body motions. Indeed, in conventional finite elasticity theory, it is known that invariance of the strain-energy function under superposed rigid-body motions is equivalent to symmetry of the Cauchy stress [9].

This issue leads us to consider the transformation rules for the elastic and plastic deformations under superposed rigid-body motions. In a way, this question is moot if we understand $\mathcal{M}$ to be a material manifold. For, $\mathcal{M}$ is then indifferent to the placement of its points in $E$ and the issue of invariance under changes of such placements does not arise [24]. The fact that $\mathbf{K}^{-1}$ maps $V$ at $\mathbf{X} \in \kappa_r$ to $T_{\mathcal{M}(p)}$ would then lead naturally to the conclusion that $\mathbf{K}$ is invariant under superposed rigid-body motions. This would then dictate, via (22), the transformation rule $\mathbf{H} \to \mathbf{QH}$, where $\mathbf{Q}(t)$ is the spatially uniform rotation in the conventional rule $\mathbf{F} \to \mathbf{QF}$. This is tacitly assumed in most works concerned with the invariance issue (e.g. [1, 26, 38, 39, 40]).

In the present work we proceed in a different manner that emphasizes the constitutive character of the constituent elastic and plastic deformations. We know from conventional theory that

$$\mathbf{F} \to \mathbf{QF} \tag{69}$$

in a superposed rigid-body motion, where $\mathbf{Q}(t) \in Orth^+$. This follows from the fact that $\mathbf{x} \to \mathbf{Qx} + \mathbf{c}$ in such a motion, with $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$ and $\mathbf{c}$ a function of $t$ alone. We also assume that

$$\mathbf{T} \to \mathbf{QTQ}^t, \quad \text{and therefore} \quad \mathbf{P} \to \mathbf{QP}. \tag{70}$$

The line of reasoning leading to (69) cannot be applied to $\mathbf{H}$ and $\mathbf{K}$ because there is no position field in $\mathcal{M}$ associated with material points $p$. Instead, we appeal to the aforementioned result in finite-elasticity theory and define superposed rigid-body motions by the requirement that $W(=\hat{W})$ have the same value at any two $\mathbf{H}$ related by a superposed rigid-body motion. Let $\mathbf{H}_1(t)$ and $\mathbf{H}_2(t)$ be two elastic deformations so related and define $\mathbf{Z}(t) = \mathbf{H}_2\mathbf{H}_1^{-1}$. We require that $\hat{W}(\mathbf{H}_1^t\mathbf{Z}^t\mathbf{Z}\mathbf{H}_1) = \hat{W}(\mathbf{H}_1^t\mathbf{H}_1)$ for $\mathbf{H}_1 \in Lin$ with $J_{H_1} > 0$. In particular, then, $\hat{W}(\mathbf{Z}^t\mathbf{Z}) = \hat{W}(\mathbf{I})$. Our constitutive hypotheses imply that $\hat{W}(\mathbf{Z}^t\mathbf{Z}) > \hat{W}(\mathbf{I})$ if $\mathbf{Z}^t\mathbf{Z} \neq \mathbf{I}$. The two statements are reconciled only if $\mathbf{Z}^t\mathbf{Z} = \mathbf{I}$ and it follows, since $J_Z > 0$, that $\mathbf{Z} \in Orth^+$. Therefore, in a superposed rigid motion,

$$\mathbf{H} \to \mathbf{Q}_H\mathbf{H}, \tag{71}$$

where $\mathbf{Q}_H$ is a rotation. Since the argument is local, this rotation may depend on $\mathbf{x}$ (or $\mathbf{X}$) in addition to $t$. It follows immediately from (71) that $\mathbf{C}_H$, $\hat{W}(\mathbf{C}_H)$ and $\mathbf{S}(\mathbf{C}_H)$ are invariant under superposed rigid motions.

To obtain the transformation rule for the plastic deformation $\mathbf{K}$, we assume that superposed rigid motions do not generate dissipation, so that the dissipations associated with any two motions related by a superposed rigid-body motion are identical. Clearly $\mathcal{E}$ is invariant under superposed rigid motions. This can be seen from (58) and the invariance of $\Psi$, which is implied by that of $W$ and $J_K$, the latter following from (22), (69) and (71). Further, from (48), (60) and (67) we have

$$\mathcal{E}' = \hat{W}(\mathbf{C}_H)\mathbf{I} - \mathbf{C}_H\mathbf{S}(\mathbf{C}_H), \tag{72}$$

which is also invariant. Suppose $\mathbf{K}_1(t)$ and $\mathbf{K}_2(t)$ are related by a superposed rigid-body motion and let $\mathbf{Z}(t) = \mathbf{K}_2\mathbf{K}_1^{-1}$. We assume the superposed rigid motion to commence at time $t_0$ so that $\mathbf{Z}(t_0) = \mathbf{I}$. If $D_1 = J_{K_1}^{-1}\mathcal{E}' \cdot \mathbf{K}_1^{-1}\dot{\mathbf{K}}_1$ is the dissipation associated with $\mathbf{K}_1$, then the dissipation $D_2$ associated with $\mathbf{K}_2$ satisfies

$$J_{K_2}D_2 = J_{K_1}D_1 + \mathcal{E}' \cdot \mathbf{K}_1^{-1}\mathbf{Z}^{-1}\dot{\mathbf{Z}}\mathbf{K}_1. \tag{73}$$

Invoking the invariance of $J_K$ and the assumed invariance of the dissipation then yields

$$\mathcal{E}' \cdot \mathbf{K}_1^{-1}\mathbf{Z}^{-1}\dot{\mathbf{Z}}\mathbf{K}_1 = 0, \tag{74}$$

for any plastic deformation $\mathbf{K}_1$. To obtain a necessary condition we set $\mathbf{K}_1 = c\mathbf{I}$, where $c > 0$, yielding $\mathcal{E}' \cdot \mathbf{Z}^{-1}\dot{\mathbf{Z}} = 0$. Hypothesis (63) is easily seen to be equivalent to the statement:

$$\dot{\mathbf{K}} \neq \mathbf{0} \quad \text{if and only if} \quad \mathcal{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}} > 0. \tag{75}$$

It follows that $\dot{\mathbf{Z}}$ vanishes and hence that $\mathbf{Z}(t) = \mathbf{Z}(t_0) = \mathbf{I}$. This is also sufficient for (74) and for the invariance of the dissipation. Thus, $\mathbf{K}_2 = \mathbf{K}_1$ and $\mathbf{K}$ is invariant under superposed rigid motions, i.e.

$$\mathbf{K} \to \mathbf{K}. \tag{76}$$

As a corollary, we then have $\mathbf{Q}_H = \mathbf{Q}(t)$, implying that $\mathbf{Q}_H$ is spatially uniform.

In addition to furnishing the transformation rules for the elastic and plastic deformations under superposed rigid motions, the strong dissipation hypothesis and our constitutive hypotheses on the elastic response also imply that plastic evolution ceases in the absence of elastic distortion. For, if $\mathbf{C}_H = \mathbf{I}$ then $\hat{W}$ and $\mathbf{S}$ vanish; therefore $\mathcal{E}'$ and $\mathcal{E}$ vanish, $D = 0$ and (63) yields $\dot{\mathbf{K}} = \mathbf{0}$.

## 7. Material symmetry

The function $W(\mathbf{H})$ is subject to restrictions imposed by material symmetry. These are of the kind one finds in conventional finite elasticity theory and are crucial to the understanding of elastic/plastic response. Accordingly, a brief review of the concept is appropriate before proceeding. Thus, if two local configurations $\kappa_{i_1}$ and $\kappa_{i_2}$ are used to describe the stress $\mathbf{T}$ at a material point in $\kappa_t$, then

$$\mathbf{T} = (W_1)_{\mathbf{H}_1}(\mathbf{H}_1^*)^{-1} \quad \text{and} \quad \mathbf{T} = (W_2)_{\mathbf{H}_2}(\mathbf{H}_2^*)^{-1}, \tag{77}$$

where $W_1(\mathbf{H}_1)$ and $W_2(\mathbf{H}_2)$ are the associated strain-energy functions. These equations are identical to (12), the role played there by $\mathbf{F}$ now being assumed by $\mathbf{H}$. Accordingly, if $\mathbf{A}$ is a map from $\kappa_{i_1}$ to $\kappa_{i_2}$, then

$$\mathbf{H}_1 = \mathbf{H}_2\mathbf{A}, \tag{78}$$

and if $\mathbf{A}$ is fixed at the material point $p$, then consistency between the two expressions for $\mathbf{T}$ requires that (cf. (13))

$$W_1(\mathbf{H}_1) = J_A W_2(\mathbf{H}_2). \tag{79}$$

This formula specifies the change in the form of the strain-energy function induced by any local time-independent change of reference at a given material point.

Suppose now that there exists a local change of reference $\mathbf{G}_1$, with $J_{G_1} = 1$, such that $W_2(\mathbf{H}) = W_1(\mathbf{H})$ with $J_H > 0$; the two local references then respond identically to a given deformation. Using (78), we find that

$$W_1(\mathbf{H}) = W_1(\mathbf{H}\mathbf{G}_1). \tag{80}$$

It is well known that the set of all such $\mathbf{G}_1$ is a group $\mathcal{G}_1$, say, the *symmetry group* associated with $\kappa_{i_1}$. If the body is materially uniform, then $W_1(\mathbf{H})$ does not depend explicitly on $p \in B$ (or on $\mathbf{X} \in \kappa_r$). This restriction is satisfied by requiring that $\mathbf{G}_1$ be independent of $p \in B$ [15, 41].

Combining (79) with (80), we have

$$J_A W_2(\mathbf{H}) = W_1(\mathbf{H}\mathbf{A}) = W_1(\mathbf{H}\mathbf{A}\mathbf{G}_1) = J_A W_2(\mathbf{H}\mathbf{A}\mathbf{G}_1\mathbf{A}^{-1}). \tag{81}$$

In other words,

$$W_2(\mathbf{H}) = W_2(\mathbf{H}\mathbf{G}_2), \quad \text{with} \quad \mathbf{G}_2 = \mathbf{A}\mathbf{G}_1\mathbf{A}^{-1}, \tag{82}$$

which is Noll's Rule $\mathcal{G}_2 = \mathbf{A}\mathcal{G}_1\mathbf{A}^{-1}$ relating the symmetry groups of the two local references.

We have seen in Section 2 that our constitutive hypotheses determine the placements of stress-free local equilibrium configurations in $E$ modulo orientation and translation. Thus, if $\kappa_{i_1}$ is a local relaxed configuration, then any $\kappa_{i_2}$ is also such a configuration provided that the transformation $\mathbf{A}$ from $\kappa_{i_1}$ to $\kappa_{i_2}$ is a rotation. Further, $\mathcal{G}_1$ is a subgroup of the orthogonal group if and only if the same is true of $\mathcal{G}_2$. Any $\mathbf{G}_2 \in \mathcal{G}_2$ is obtained simply by rotating some $\mathbf{G}_1 \in \mathcal{G}_1$ by $\mathbf{A}$ to obtain $\mathbf{G}_2 = \mathbf{A}\mathbf{G}_1\mathbf{A}^t$. For example, if $\mathbf{e}_i; i = 1, 2, 3$ are the orthonormal axes of a cubic lattice in $\kappa_{i_1}$, then the 180° rotation $\mathbf{G}_1 = 2\mathbf{e}_3 \otimes \mathbf{e}_3 - \mathbf{I}$ about $\mathbf{e}_3$ maps the lattice to itself and thus belongs to $\mathcal{G}_1$. The corresponding element of $\mathcal{G}_2$ is given by $\mathbf{G}_2 = 2\mathbf{e}_3' \otimes \mathbf{e}_3' - \mathbf{I}$, where $\mathbf{e}_i' = \mathbf{A}\mathbf{e}_i$.

This result is of the greatest importance for the practical implementation of the theory. It implies that the symmetry group $\mathcal{G}_1$ for the local stress-free $\kappa_{i_1}$ may be fixed once and for all, provided that this group is a sub-group of the orthogonal group. Then, given the response function $W_1(\mathbf{H})$, we generate the response function relative to any relaxed local configuration $\kappa_{i_2}$ by setting $W_2(\mathbf{H}) = W_1(\mathbf{HA})$, where $\mathbf{A}$ is a suitable rotation. By construction, all such configurations are equivalent insofar as the computation of the stress is concerned. The same issue is discussed from a different viewpoint in [1].

For example, if the material in configuration $\kappa_i$ exhibits cubic symmetry, and if the elastic strain is sufficiently small to justify a quadratic approximation to the strain-energy function, then [42]

$$\hat{W} = \tfrac{1}{2}C_1(E_{11} + E_{22} + E_{33})^2 + C_2(E_{11}E_{22} + E_{11}E_{33} + E_{22}E_{33}) + C_3(E_{12}^2 + E_{13}^2 + E_{23}^2), \tag{83}$$

where $C_i; i = 1, 2, 3$ are material constants, $E_{ij} = \mathbf{E} \cdot Sym(\mathbf{e}_i \otimes \mathbf{e}_j)$, $\{\mathbf{e}_i\}$ is a basis of orthonormalized vectors aligned with the cube axes, and

$$\mathbf{E} = \tfrac{1}{2}(\mathbf{C}_H - \mathbf{I}) \tag{84}$$

is the elastic strain. The linear and quadratic invariants of $\mathbf{E}$ are common to each of the five subclasses of cubic symmetry [42]. Accordingly, (83) applies to all kinds of cubic symmetry. From (68) we then obtain

$$\begin{aligned} \mathbf{S} \;=\;& C_1(tr\mathbf{E})\mathbf{I} + C_2[(E_{22} + E_{33})\mathbf{e}_1 \otimes \mathbf{e}_1 + (E_{11} + E_{33})\mathbf{e}_2 \otimes \mathbf{e}_2 + (E_{11} + E_{22})\mathbf{e}_3 \otimes \mathbf{e}_3] \\ & + C_3[E_{12}(\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1) + E_{13}(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) + E_{23}(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2)]. \end{aligned} \tag{85}$$

Our requirement that $\hat{W}$ be a convex function of $\mathbf{C}_H$ is satisfied if and only if it is a convex function of $\mathbf{E}$. In the quadratic case this in turn is satisfied if and only if the energy is a positive-definite function of $\mathbf{E}$. To construct necessary conditions for this, we set all $E_{ij} = 0$ except $E_{12}(= E_{21})$. The resulting inequality can then be satisfied only if $C_3 > 0$, which in turn ensures that the final quadratic form in (83) is positive definite. Next, we set all off-diagonal components $E_{ij}$ to zero, along with $E_{33}$. We then require

$$\tfrac{1}{2}C_1(E_{11} + E_{22})^2 + C_2 E_{11}E_{22} > 0 \tag{86}$$

for all $E_{11}$, $E_{22}$. For this it is necessary and sufficient that $C_1 > 0$ and $C_2 \in (-2C_1, 0)$. Necessary conditions for positive-definiteness are thus given by

$$C_1 > 0, \quad C_3 > 0, \quad -2C_1 < C_2 < 0. \tag{87}$$

To derive sufficient conditions we write (83) in the form

$$\hat{W} = P(E_{11}, E_{22}) + P(E_{11}, E_{33}) + P(E_{22}, E_{33}) + C_3(E_{12}^2 + E_{13}^2 + E_{23}^2), \tag{88}$$

where

$$P(A, B) = \tfrac{1}{4}C_1(A^2 + B^2) + (C_1 + C_2)AB. \tag{89}$$

Sufficient conditions for positive-definiteness are $C_3 > 0$ and $P(A, B) > 0$, which holds if and only if $C_1 > 0$ and $C_1^2 > 4(C_1 + C_2)^2$. The latter are equivalent to $C_1/2 > |C_1 + C_2|$. Taken together we have

$$C_1 > 0, \quad C_3 > 0, \quad -\tfrac{3}{2}C_1 < C_2 < -\tfrac{1}{2}C_1. \tag{90}$$

From the foregoing discussion it is clear that, in the presence of convexity, the response functions relative to any other stress-free local configuration are obtained from those given simply by substituting $\mathbf{e}'_i = \mathbf{A}\mathbf{e}_i$ in place of $\mathbf{e}_i$, where $\mathbf{A}$ is a suitable rotation. Accordingly, since these configurations are, by construction, equivalent insofar as the computation of the stress in $\kappa_t$ is concerned, we may fix the basis $\{\mathbf{e}_i\}$, and hence the symmetry group $\mathcal{G}_{\kappa_i}$, once and for all. For example, we may identify $\mathbf{e}_i$ with their values in some known configuration of the body, which may then serve as a reference configuration $\kappa_r$. This is not to say that we identify $\kappa_i$ with $\kappa_r$; rather, we simply require that $\mathcal{G}_{\kappa_i}$ be insensitive to plastic flow, as suggested by the physics of crystal slip [14, 43]. Similar ideas are imposed *a priori* as part of the definition of plastic deformation in [1, 38, 39].

In the isotropic case the quadratic approximation to the strain-energy function and the associated expression for the stress are, of course, well known. Thus,

$$\hat{W} = \tfrac{1}{2}\lambda(tr\mathbf{E})^2 + \mu\mathbf{E}\cdot\mathbf{E} \quad \text{and} \quad \mathbf{S} = \lambda(tr\mathbf{E})\mathbf{I} + 2\mu\mathbf{E}, \tag{91}$$

where $\lambda$ and $\mu$ are the Lamé moduli. Necessary and sufficient conditions for convexity are that $\mu > 0$ and $\lambda + \frac{2}{3}\mu > 0$.

## 8. Flow and yield

To complete the model we require a flow rule for the evolution of plastic deformation $\mathbf{K}$. In view of the structure of the dissipation inequality (63), it is natural to consider rules of the form

$$\mathcal{F}(\mathbf{K}, \dot{\mathbf{K}}, \mathbf{H}, \dot{\mathbf{H}}, \mathcal{E}, \mathcal{E}^{\cdot}, \boldsymbol{\alpha}_r) = \mathbf{0}, \tag{92}$$

where $\mathcal{F}$ is a tensor-valued function. It is assumed, in line with our assumption of material uniformity, that this function does not depend explicitly on $p$. The presence of the dislocation density in flow rules and yield criteria may be motivated by G.I. Taylor's formula giving the flow stress on a slip system as a function of the density of the relevant type of dislocation [26, 43, 44, 45]. Thus, dislocation density is expected to play a role in yield and flow whenever work hardening is in evidence.

### (a) *Invariance requirements*

Following Epstein [7], we impose the requirement that equation (92) be invariant under compatible changes of the reference configuration $\kappa_r$. The reason for this is that the choice of reference is in principle a matter of convenience and hence irrelevant to the physical processes under study. Precisely the same viewpoint was adopted in the derivation of (13) by invoking the insensitivity of the Cauchy stress to the choice of reference.

To effect this program in the present context, we observe from (58) that the function of $\mathbf{H}$, $\mathbf{K}$ and $\mathcal{E}$ defined by

$$\mathcal{E}^* \doteq J_F^{-1}\mathbf{F}^{-t}\mathcal{E}\mathbf{F}^t \tag{93}$$

satisfies

$$\mathcal{E}^* = \psi\mathbf{I} - \mathbf{T}, \tag{94}$$

where $\mathbf{T}$ is the Cauchy stress and $\psi = J_F^{-1}\Psi$ is the energy per unit volume of $\kappa_t$. These are insensitive to the choice of reference configuration. Accordingly, if $\kappa_{r_1}$ and $\kappa_{r_2}$ are two reference configurations related by a compatible deformation, then the associated Eshelby tensors are

$$\mathcal{E}_1 = J_{F_1}\mathbf{F}_1^t\mathcal{E}^*\mathbf{F}_1^{-t} \quad \text{and} \quad \mathcal{E}_2 = J_{F_2}\mathbf{F}_2^t\mathcal{E}^*\mathbf{F}_2^{-t}, \tag{95}$$

respectively, where $\mathbf{F}_1 = \mathbf{F}_2\mathbf{R}$ and $\mathbf{R}$ is the gradient of the map from $\kappa_{r_1}$to $\kappa_{r_2}$, this following on use of (30) with $\mathbf{H}_1 = \mathbf{H}_2$. Therefore [7],

$$\mathcal{E}_2 = J_R^{-1}\mathbf{R}^{-t}\mathcal{E}_1\mathbf{R}^t. \tag{96}$$

The assumed insensitivity of (92) to the choice of reference then implies that

$$\begin{aligned}
&\mathcal{F}(\mathbf{K}_1,\, \dot{\mathbf{K}}_1,\, \mathbf{H}_1,\, \dot{\mathbf{H}}_1,\, \mathcal{E}_1,\, \mathcal{E}_1^{\cdot},\, \boldsymbol{\alpha}_{r_1}) \\
=\;& \mathcal{F}(\mathbf{K}_2,\, \dot{\mathbf{K}}_2,\, \mathbf{H}_2,\, \dot{\mathbf{H}}_2,\, \mathcal{E}_2,\, \mathcal{E}_2^{\cdot},\, \boldsymbol{\alpha}_{r_2}) \\
=\;& \mathcal{F}(\mathbf{R}\mathbf{K}_1,\, \mathbf{R}\dot{\mathbf{K}}_1,\, \mathbf{H}_1,\, \dot{\mathbf{H}}_1,\, J_R^{-1}\mathbf{R}^{-t}\mathcal{E}_1\mathbf{R}^t,\, J_R^{-1}\mathbf{R}^{-t}\mathcal{E}_1^{\cdot}\mathbf{R}^t,\, J_R^{-1}\mathbf{R}\boldsymbol{\alpha}_{r_1}),
\end{aligned} \tag{97}$$

where $(27)_1$ and (31) have been used and we have assumed the *function* $\mathcal{F}$ to be invariant. A necessary condition follows by setting $\mathbf{R}$ equal to the instantaneous local value of $\mathbf{K}_1^{-1}$ [7]. This is permissible because (92) is presumed to hold at a fixed instant and a fixed material point. This means that the identification of $\mathbf{R}$ with $\mathbf{K}_1^{-1}$ in (97) imposes no relationship between their time derivatives or their gradients. In particular, the fact that $\mathbf{R}$ is compatible and independent of $t$ (when regarded as a function of $\mathbf{X}$ and $t$), whereas $\mathbf{K}_1^{-1}$ is generally incompatible and dependent on $t$, is irrelevant insofar as (97) is concerned. We then have

$$\mathcal{F}(\mathbf{K},\, \dot{\mathbf{K}},\, \mathbf{H},\, \dot{\mathbf{H}},\, \mathcal{E},\, \mathcal{E}^{\cdot},\, \boldsymbol{\alpha}_r) = \mathcal{F}(\mathbf{I},\, \mathbf{K}^{-1}\dot{\mathbf{K}},\, \mathbf{H},\, \dot{\mathbf{H}},\, \mathcal{E}',\, J_K\mathbf{K}^t\mathcal{E}^{\cdot}\mathbf{K}^{-t},\, \boldsymbol{\alpha}), \tag{98}$$

where $(28)_1$ has been used and $\mathcal{E}'$ is defined by (59). Now, it is straightforward to show that

$$J_K\mathbf{K}^t\mathcal{E}^{\cdot}\mathbf{K}^{-t} = (\mathcal{E}')^{\cdot} + \mathcal{E}'(\mathbf{K}^{-1}\dot{\mathbf{K}})^t - (\mathbf{K}^{-1}\dot{\mathbf{K}})^t\mathcal{E}' - \mathcal{E}'tr(\mathbf{K}^{-1}\dot{\mathbf{K}}), \tag{99}$$

so that the functional dependence on $J_K\mathbf{K}^t\mathcal{E}^{\cdot}\mathbf{K}^{-t}$ may be eliminated in favor of $(\mathcal{E}')^{\cdot}$ and other arguments of $\mathcal{F}$. Further, if we impose the invariance of the *function* $\mathcal{F}$ under superposed rigid-body motions then it is unaffected by substituting $\mathbf{Q}(t)\mathbf{H}$ in place of $\mathbf{H}$. Equating $\mathbf{Q}^t$ identically to the rotation in the polar factorization of $\mathbf{H}$, we then have

$$\mathcal{F}(\mathbf{I},\, \mathbf{K}^{-1}\dot{\mathbf{K}},\, \mathbf{H},\, \dot{\mathbf{H}},\, \mathcal{E}',\, J_K\mathbf{K}^t\mathcal{E}^{\cdot}\mathbf{K}^{-t},\, \boldsymbol{\alpha}) = \mathcal{G}(\mathbf{K}^{-1}\dot{\mathbf{K}},\, \mathbf{C}_H,\, \dot{\mathbf{C}}_H,\, \mathcal{E}',\, (\mathcal{E}')^{\cdot},\, \boldsymbol{\alpha}), \tag{100}$$

for some function $\mathcal{G}$, where the invariance of $\boldsymbol{\alpha}$ under superposed rigid motions has been used, this following from the fact that $\boldsymbol{\alpha}$ is invariant under compatible variations of $\kappa_t$ (Section 3 and [26]). Its further invariance under compatible variations of $\kappa_r$, together with

$$\mathcal{E}' = J_H\mathbf{H}^t\mathcal{E}^*\mathbf{H}^{-t}, \tag{101}$$

may then be used to show that (100) yields $(97)_1$ for any time-independent $\mathbf{R}$, so that (100) is necessary and sufficient for the stated invariance, provided that the *function* $\mathcal{G}$ is invariant. We note from (72) that the fourth and fifth arguments of $\mathcal{G}$ are determined by the second and third and may therefore be eliminated. Imposing (92), we consider special cases of (100) of the form

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{H}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}). \tag{102}$$

Our constitutive hypotheses on the strain-energy function $\hat{W}(\mathbf{C}_H)$ ensure that the relation between $\mathbf{C}_H$ and $\mathbf{S} = 2Sym\hat{W}_{\mathbf{C}_H}$ is one-to-one. Accordingly, $\mathbf{S}$ and $\dot{\mathbf{S}}$ may replace $\mathbf{C}_H$ and $\dot{\mathbf{C}}_H$ as arguments of $\mathcal{H}$.

(b) *Plastic spin*

We observe from (72) that $\mathbf{M}(\mathbf{C}_H) \in Sym$, where

$$\mathbf{M}(\mathbf{C}_H) = \mathcal{E}'\mathbf{C}_H. \tag{103}$$

To embed this fact in the model, we write the dissipation (cf. (61)) in the form

$$J_K D = \mathbf{M} \cdot \mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1}. \tag{104}$$

Hypothesis (63) is then equivalent to the statement

$$\dot{\mathbf{K}} \neq \mathbf{0} \quad \text{if and only if} \quad \mathbf{M} \cdot \mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1} > 0. \tag{105}$$

It follows immediately that $\dot{\mathbf{K}}$ vanishes if $\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1} \in Skw$. In other words, the latter does not correspond to a *bona fide* evolution of plasticity. Conversely, if $\dot{\mathbf{K}} \neq \mathbf{0}$ then $\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1}$ is not skew. This of course should not be construed to mean that that latter is symmetric. However, it does beg the question of how the skew part of $\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1}$ should be interpreted. This is the issue of *plastic spin*, which is of significant ongoing concern in the plasticity literature (e.g. [1, 40, 46]). To address it, we exploit the latitude afforded by the constitutive character of $\mathbf{K}$ and adopt the *constitutive* assumption

$$\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1} \in Sym. \tag{106}$$

In effect, this resolves the issue simply by requiring that indeterminate variables vanish.

The flow rule (102) simplifies accordingly. We have

$$\mathbf{K}^{-1}\dot{\mathbf{K}}\mathbf{C}_H^{-1} = \mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}), \tag{107}$$

where

$$\mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha}) = \mathcal{H}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha})\mathbf{C}_H^{-1} \in Sym. \tag{108}$$

The plastic deformation then satisfies

$$\dot{\mathbf{K}} = \mathbf{K}\mathcal{S}(\mathbf{C}_H, \dot{\mathbf{C}}_H, \boldsymbol{\alpha})\mathbf{C}_H; \quad \mathbf{K}(t_0) = \mathbf{K}_0, \tag{109}$$

with $\boldsymbol{\alpha}$ given by $(28)_1$.

The specialization to rate-independent response is of particular interest in applications. In this case we require the flow rule to be insensitive to the time scale, so that $\mathcal{S}$ is homogeneous of degree one in its second argument, i.e.

$$\mathcal{S}(\mathbf{C}_H,\, \lambda\dot{\mathbf{C}}_H,\, \boldsymbol{\alpha}) = \lambda\mathcal{S}(\mathbf{C}_H,\, \dot{\mathbf{C}}_H,\, \boldsymbol{\alpha}) \quad \text{for all} \quad \lambda \in \mathbb{R}. \tag{110}$$

Differentiating with respect to $\lambda$ and evaluating the result at $\lambda = 0$ furnishes the necessary and sufficient condition

$$\mathcal{S}(\mathbf{C}_H,\, \dot{\mathbf{C}}_H,\, \boldsymbol{\alpha}) = \mathcal{M}(\mathbf{C}_H,\, \boldsymbol{\alpha})[\dot{\mathbf{C}}_H], \tag{111}$$

where $\mathcal{M}$ is a fourth-order tensor possessing the major symmetry $\mathbf{A} \cdot \mathcal{M}[\mathbf{B}] = \mathbf{B} \cdot \mathcal{M}[\mathbf{A}]$ for all $\mathbf{A}, \mathbf{B} \in$ *Sym*.

(c) *Material symmetry*

It is obvious from its structure that the function $\mathcal{S}$ (or $\mathcal{H}$) depends on the local configuration $\kappa_i$. We are concerned with material symmetry and thus with the question of how the flow rule transforms under variations of these configurations. The role of material symmetry in this context is discussed in the comprehensive review by Cleja-Tigiou and Soos [1] and independently by Epstein [7]. Thus, consider a map from $\kappa_{i_1}$ to $\kappa_{i_2}$, as in Section 7. Assume $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$ to be given. Imposing (22) and (78) at fixed $\mathbf{F}$, we have

$$\mathbf{K}_1 = \mathbf{K}_2\mathbf{A}. \tag{112}$$

Writing (109) for both local configurations, we are then led, using obvious notation, to the rule

$$\mathcal{S}_2(\mathbf{C}_{H_2},\, \dot{\mathbf{C}}_{H_2},\, \boldsymbol{\alpha}_2) = \mathbf{A}\mathcal{S}_1(\mathbf{C}_{H_1},\, \dot{\mathbf{C}}_{H_1},\, \boldsymbol{\alpha}_1)\mathbf{A}^t, \tag{113}$$

where, for $\mathbf{A}$ fixed at $p$, as in Section 7,

$$\mathbf{C}_{H_1} = \mathbf{A}^t\mathbf{C}_{H_2}\mathbf{A} \quad \text{and} \quad \dot{\mathbf{C}}_{H_1} = \mathbf{A}^t\dot{\mathbf{C}}_{H_2}\mathbf{A}. \tag{114}$$

We use $(28)_1$ to relate $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$. Thus,

$$\boldsymbol{\alpha}_1 = J_{K_1}\mathbf{K}_1^{-1}Curl\mathbf{K}_1^{-1} = J_A J_{K_2}\mathbf{A}^{-1}\mathbf{K}_2^{-1}Curl(\mathbf{A}^{-1}\mathbf{K}_2^{-1}). \tag{115}$$

If the change of local reference is uniform, in the sense that $\mathbf{A}$ is independent of $p$ (hence, of $\mathbf{X}$), we have [26]

$$Curl(\mathbf{A}^{-1}\mathbf{K}_2^{-1}) = (Curl\mathbf{K}_2^{-1})\mathbf{A}^{-t}, \tag{116}$$

yielding

$$\boldsymbol{\alpha}_1 = J_A\mathbf{A}^{-1}\boldsymbol{\alpha}_2\mathbf{A}^{-t}. \tag{117}$$

Thus, if the function $\mathcal{S}_1$ is known, then $\mathcal{S}_2$ is generated by the formula

$$\mathcal{S}_2(\mathbf{C}_H,\, \dot{\mathbf{C}}_H,\, \boldsymbol{\alpha}) = \mathbf{A}\mathcal{S}_1(\mathbf{A}^t\mathbf{C}_H\mathbf{A},\, \mathbf{A}^t\dot{\mathbf{C}}_H\mathbf{A},\, J_A\mathbf{A}^{-1}\boldsymbol{\alpha}\mathbf{A}^{-t})\mathbf{A}^t. \tag{118}$$

Since the local configurations $\kappa_{i_1}$ and $\kappa_{i_2}$ are stress-free by definition, our constitutive hypotheses give $\mathbf{A} \in Orth^+$, affording the simplification

$$\mathcal{S}_2(\mathbf{C}_H,\, \dot{\mathbf{C}}_H,\, \boldsymbol{\alpha}) = \mathbf{A}\mathcal{S}_1(\mathbf{A}^t\mathbf{C}_H\mathbf{A},\, \mathbf{A}^t\dot{\mathbf{C}}_H\mathbf{A},\, \mathbf{A}^t\boldsymbol{\alpha}\mathbf{A})\mathbf{A}^t. \tag{119}$$

Suppose now that the transformation is such that both local references respond identically. Let $\mathbf{G}_1$ be such a transformation. Then the functions $\mathcal{S}_1$ and $\mathcal{S}_2$ coincide, and (119) furnishes

$$\mathbf{G}_1^t\mathcal{S}_1(\mathbf{C}_H,\, \dot{\mathbf{C}}_H,\, \boldsymbol{\alpha})\mathbf{G}_1 = \mathcal{S}_1(\mathbf{G}_1^t\mathbf{C}_H\mathbf{G}_1,\, \mathbf{G}_1^t\dot{\mathbf{C}}_H\mathbf{G}_1,\, \mathbf{G}_1^t\boldsymbol{\alpha}\mathbf{G}_1). \tag{120}$$

Here we identify $\mathbf{G}_1$ with any element of $\mathcal{G}_1$, the symmetry group associated with $\kappa_{i_1}$. The restriction to uniform $\mathbf{A}$ (hence uniform $\mathbf{G}_1$) is due to our prescription for enforcing the condition of material uniformity in Section 7.

A straightforward but involved calculation based on (118) and (120) furnishes the analog of Noll's Rule for plastic flow, but we do not record this here.

In practice, given $\mathcal{G}_1$, (120) is solved by regarding $\mathcal{S}$ as a function of three symmetric tensors and one vector [47]. This reduction is achieved by writing $\mathcal{S}$ as a function of $Sym\boldsymbol{\alpha}$ and $Skw\boldsymbol{\alpha}$. If $\mathbf{a}$ is the axial vector of $Skw\boldsymbol{\alpha}$, then $\mathbf{G}^t(Skw\boldsymbol{\alpha})\mathbf{G}$ may be replaced by $\mathbf{G}^t\mathbf{a}$ in the statement of material symmetry, for any $\mathbf{G} \in \mathcal{G}_1 \subset Orth^+$. To see this we observe that for any vector $\mathbf{u}$,

$$\mathbf{G}^t\mathbf{a} \times \mathbf{G}^t\mathbf{u} = \mathbf{G}^t(\mathbf{a} \times \mathbf{u}) = \mathbf{G}^t(Skw\boldsymbol{\alpha})\mathbf{u} = [\mathbf{G}^t(Skw\boldsymbol{\alpha})\mathbf{G}](\mathbf{G}^t\mathbf{u}), \tag{121}$$

so that $\mathbf{G}^t\mathbf{a}$ is the axial vector of $\mathbf{G}^t(Skw\boldsymbol{\alpha})\mathbf{G}$. With this simplification, the problem of solving (120) for the canonical form of the response function is tractable [47]. It is eased considerably in the rate independent case in which the functional dependence on $\dot{\mathbf{C}}_H$ is linear.

In the case of isotropy, $\mathbf{C}_H$ commutes with $\mathbf{S}(\mathbf{C}_H)$, so that $\mathcal{E}' \in Sym$. It follows from (63) and the argument leading from (105) to (106) that if $\dot{\mathbf{K}} \neq \mathbf{0}$, then $\mathbf{K}^{-1}\dot{\mathbf{K}} \in Sym$, and thus from (107) that $\mathbf{C}_H$ also commutes with $\mathcal{S}$. This means that $\mathcal{H} \in Sym$, where $\mathcal{H}$ is now a hemitropic function of its arguments. However, the present model, in which dislocation density figures in the determination of the state of the material, is not appropriate in the case of isotropy. This is due to the degree of freedom $\mathbf{H} \to \mathbf{HG}$ afforded by material symmetry. If $\mathbf{G}$ belongs to a continuous group, as in the case of isotropy or transverse isotropy, then the dislocation density is highly non-unique and is therefore not a state variable. The issue is discussed in [15; Thm. 8] and investigated in [41]. There is no such difficulty in the case of a discrete group, however. In the isotropic case, Riemannian curvature derived from the plastic strain furnishes a unique measure of defectiveness of the material. The associated theory entails significant complications vis à vis that considered here [48].

Conventionally, flow is considered to be possible only if the material is in a state of yield. This is enforced by requiring the pertinent variables to belong to a certain manifold, assumed here to be expressible in the form

$$f(\mathbf{K},\, \mathbf{H},\, \mathcal{E},\, \boldsymbol{\alpha}_r) = 0, \tag{122}$$

which is preserved by compatible changes of reference configuration and by superposed rigid-body motions. From the foregoing it is immediate that such invariance yields the reduced form

$$f = g(\mathbf{C}_H,\, \boldsymbol{\alpha}), \tag{123}$$

which is subject to the restriction

$$g(\mathbf{C}_H, \boldsymbol{\alpha}) = g(\mathbf{G}^t\mathbf{C}_H\mathbf{G}, \mathbf{G}^t\boldsymbol{\alpha}\mathbf{G}) \tag{124}$$

due to material symmetry, this being meaningful only if the symmetry group is discrete. Further, we assume the response to be elastic, in the sense that $\dot{\mathbf{K}} = \mathbf{0}$, for all $\mathbf{C}_H$ and $\boldsymbol{\alpha}$ such that $g < 0$. This *elastic range* is assumed to contain $\mathbf{C}_H = \mathbf{I}$, for consistency with our earlier finding that plastic flow vanishes in the absence of elastic distortion.

Often further constitutive hypotheses are introduced which lead to a relationship between the yield function and flow rule. We consider these and their implications elsewhere in the context of specific applications of the general theory.

The initial-boundary-value problem for $\mathbf{x} = \boldsymbol{\chi}(\mathbf{X}, t)$ is specified by substituting the Piola stress (cf. $(3)_2$, (48), (49), (67))

$$\mathbf{P} = (\nabla\boldsymbol{\chi})\boldsymbol{\Pi} \tag{125}$$

into $(3)_1$, where

$$\boldsymbol{\Pi} = J_K^{-1}\mathbf{K}[\mathbf{S}(\mathbf{C}_H)]\mathbf{K}^t, \quad \text{with} \quad \mathbf{C}_H = \mathbf{K}^t(\nabla\boldsymbol{\chi})^t(\nabla\boldsymbol{\chi})\mathbf{K}, \tag{126}$$

is the 2nd Piola-Kirchhoff stress relative to $\kappa_r$ and $\mathbf{K}$ is the solution to (109).

(d) *Small elastic strain*

If the elastic strain is small, then $\mathbf{S} = O(|\mathbf{E}|)$ and, from (72) and (103),

$$\mathbf{M},\, \mathcal{E}' = -\mathbf{S} + o(|\mathbf{E}|), \tag{127}$$

so that $\mathbf{M}$ and $\mathcal{E}'$ agree to leading order. To obtain an estimate for the right-hand side of (109), we use (84) to define

$$\mathcal{S}'(\mathbf{E}, \dot{\mathbf{E}}, \boldsymbol{\alpha}) = \mathcal{S}(\mathbf{I} + 2\mathbf{E}, 2\dot{\mathbf{E}}, \boldsymbol{\alpha}). \tag{128}$$

Since $\dot{\mathbf{K}}$ vanishes in the absence of elastic distortion (Section 6), we have $\mathcal{S}'(\mathbf{0}, \dot{\mathbf{E}}, \boldsymbol{\alpha}) = \mathbf{0}$ by virtue of (107), and if $\mathcal{S}'$ is a smooth function of its first argument, (109) furnishes

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{T}(\mathbf{E}, \dot{\mathbf{E}}, \boldsymbol{\alpha}) + o(|\mathbf{E}|), \tag{129}$$

where $\mathcal{T}(\mathbf{E}, \dot{\mathbf{E}}, \boldsymbol{\alpha})$ is a *symmetric-tensor-valued* function *linear* in $\mathbf{E}$. In the rate-independent case it is also linear in $\dot{\mathbf{E}}$. Writing $\mathbf{S}(\mathbf{E})$ for the linear approximation to $\mathbf{S}$ (see, for example, (85) and $(91)_2$) we then have

$$J_K D = -\mathbf{S}(\mathbf{E}) \cdot \mathcal{T}(\mathbf{E}, \dot{\mathbf{E}}, \boldsymbol{\alpha}) + o(|\mathbf{E}|^2). \tag{130}$$

A necessary condition for strict dissipation follows on dividing by $|\mathbf{E}|^2$ and passing to the limit. Thus, if $\dot{\mathbf{K}} \neq \mathbf{0}$, then

$$\mathbf{S}(\mathbf{E}) \cdot \mathcal{T}(\mathbf{E}, \dot{\mathbf{E}}, \boldsymbol{\alpha}) < 0. \tag{131}$$

Given the one-to-one relationship between $\mathbf{S}$ and $\mathbf{E}$ implied by our constitutive assumptions, we may write

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha}) + o(|\mathbf{S}|), \tag{132}$$

in which $\mathbf{S}$ is non-dimensionalized by the largest modulus in the linear function $\mathbf{S}(\mathbf{E})$, and $\mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha}) = \mathcal{T}[\mathbf{E}(\mathbf{S}), (\mathbf{E}(\mathbf{S}))^{\cdot}, \boldsymbol{\alpha}]$ is a symmetric-tensor-valued function linear in $\mathbf{S}$ (and also in $\dot{\mathbf{S}}$ in the rate-independent case). It is then necessary that

$$\mathbf{S} \cdot \mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha}) < 0 \tag{133}$$

whenever $\dot{\mathbf{K}} \neq \mathbf{0}$. Further, since, under material symmetry, $\mathbf{E}$ and $\mathbf{S}$ transform to $\mathbf{G}^t\mathbf{E}\mathbf{G}$ and $\mathbf{G}^t\mathbf{S}\mathbf{G}$, respectively, the representation problems for $\mathcal{T}(\mathbf{E}, \dot{\mathbf{E}}, \boldsymbol{\alpha})$ and $\mathcal{R}(\mathbf{S}, \dot{\mathbf{S}}, \boldsymbol{\alpha})$ are the same as that for $\mathcal{S}$, except of course that the former are eased considerably by the linear dependence on the first arguments, or by the bilinear dependence on the first two arguments in the case of rate independence.

In the same way, if the yield function $g$ depends smoothly on its first argument, then

$$g(\mathbf{C}_H, \boldsymbol{\alpha}) = h(\mathbf{E}, \boldsymbol{\alpha}) + o(|\mathbf{E}|^2), \tag{134}$$

where $h$ contains terms linear and quadratic in $\mathbf{E}$. Our constitutive hypotheses imply that this may be written as a similar function of $\mathbf{S}$. These functions are subject to material symmetry restrictions which follow trivially from (124). Taylor's formula for the flow stress in single crystals involves a linear relationship between the square of stress and the operative dislocation density. This suggests that a linear dependence of $h$ on $\boldsymbol{\alpha}$ is relevant. Yield functions of this kind (modulo dislocation density) have recently been studied [49] and correlated with experimental data on materials having various kinds of symmetry. These may be adapted directly to the present framework by using $\mathbf{S}$ as the operative stress measure and regarding $\mathcal{G}_{\kappa_i}$ as the relevant symmetry group.

Finally, we observe that the present model, based on the idea of a stress-free manifold, does not admit *back stress* as a constitutive variable. Back stress is thought to be responsible for the Bauschinger effect [40]. Instead, back stress is regarded as residual stress arising from a dislocation density distribution and a consequent distribution of elastic strain. In principle, the residual stress field may be determined from the dislocation density distribution [14, 50] and is therefore a feature of the solution to a suitably posed initial-boundary-value problem. Its presence effectively means that the proximity of the local stress state to the yield manifold varies over the body, and thus that yield in a loaded body is non-uniformly distributed. From this point of view the Bauschinger effect is structural, rather than constitutive, in nature.

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