Mechanically equivalent elastic-plastic deformations and the problem of plastic spin

David Steigmann, Anurag Gupta

Mechanically equivalent elastic-plastic deformations and the problem of plastic spin*

David J. Steigmann[1**] and Anurag Gupta[2]

[1]Department of Mechanical Engineering
University of California
Berkeley, CA. 94720

[2]Department of Mechanical Engineering
Indian Institute of Technology
Kanpur, UP, India 208016

* *dedicated to Marcelo Epstein, in gratitude for his fundamental contributions to theoretical mechanics*

** *author to receive correspondence (steigman@me.berkeley.edu)*

Abstract: The problem of plastic spin is phrased in terms of a notion of mechanical equivalence among local relaxed configurations of an elastic/plastic crystalline solid. This idea is used to show that, without further qualification, the plastic spin may be suppressed at the constitutive level. However, the spin is closely tied to an underlying undistorted crystal lattice which, once specified, eliminates the freedom afforded by mechanical equivalence. As a practical matter a constitutive specification of plastic spin is therefore required. Suppression of plastic spin thus emerges as merely one such specification among many. Restrictions on these are derived in the case of rate-independent response.

1. Introduction

The conventional theory of crystal plasticity rests on a purely kinematical interpretation of plastic deformation according to which the rate of plastic deformation is presumed to be expressible in the form

$$\dot{\mathbf{G}}\mathbf{G}^{-1} = \sum \nu_i \mathbf{s}_i \otimes \mathbf{n}_i \tag{1}$$

as a summation of simple shear rates, in which $\mathbf{G}$ is the plastic part of the deformation gradient, ν_i are the *slips* and the $\mathbf{s}_i$ and $\mathbf{n}_i$ are orthonormal vectors specifying the i^{th} slip system. The sum ranges over the currently active slip systems. This decomposition, though virtually ubiquitous [1-4], has been criticized on the grounds that for finite deformations it cannot be associated with a sequence of simple shears unless these are restricted in a manner that is unlikely to be realized in applications [5]. In particular, the order of the sequence generally affects the overall plastic deformation, a fact which is not reflected in (1). In [6] conditions are given under which (1) yields an approximation to the deformation associated with a sequence of slips. Again it is not known if such conditions are realized in practice.

This state of affairs regarding theories based on (1) gives impetus to alternative models based purely on the continuum mechanics of crystalline media, such as those advanced in [7-10]. Here our objective is to characterize an aspect of such models - the plastic spin - which has thus far remained open to question. In conventional crystal plasticity theory, based on (1), this issue does not arise. Instead, the ν_i are determined by suitable flow rules, arranged to ensure that the response is dissipative, and the skew part of (1), in which the slip-system vectors are specified, furnishes the plastic spin.

In Section 2 we summarize the basic purely mechanical theory of elastic-plastic solids outlined in [10] and [11]. In preparation for the discussion of mechanical equivalence in Section 4, in Section 3 we split the space of tensors into the direct sum of those that contribute to plastic dissipation and *nilpotent* tensors that make no contribution. It is then shown in Section 4 that elements of the former space are mechanically equivalent to elements of the full space. This leads to the conclusion that the nilpotent plastic spin may be suppressed at the constitutive level without loss of generality. The same conclusion has been reached elsewhere [2] for the theory of isotropic elastic/plastic solids. However, implementation [3] of the theory of crystalline elastic/plastic solids relies on the *a priori* specification either of an undistorted lattice or an associated set of slip-system vectors. We show in Section 5 that when this is done the freedom to suppress the nilpotent part of the plastic evolution, afforded by the concept of mechanical equivalence, is lost. Thus, as a practical matter, constitutive equations for the plastic spin are required. These in turn depend intimately on the nature of the crystal. In Section 6 we derive restrictions on such dependence arising from ideas prevalent in the rate-independent theory [12,13], narrowing substantially the scope of those obtained previously [14,15].

The finding that plastic spin is non-negligible in principle is far from a shortcoming of the continuum theory. Rather, plastic spin affords additional freedom to fit predictions of the theory to actual data. Indeed, such freedom substantially exceeds that afforded by conventional crystal plasticity theory in which plastic spin is constrained by the structure of (1).

We use standard notation such as $\mathbf{A}^t$, $\mathbf{A}^{-1}$, $\mathbf{A}^*$, $Sym\mathbf{A}$, $Skw\mathbf{A}$, $tr\mathbf{A}$ and J_A. These are respectively the transpose, the inverse, the cofactor, the symmetric part, the skew part, the trace and the determinant of a tensor $\mathbf{A}$, regarded as a linear transformation from a three-dimensional vector space to itself, the latter being identified with the translation space of the usual three-dimensional Euclidean point space. We also use Lin to denote the linear space of second-order tensors, Lin^+ the group of tensors with positive determinant, $Orth^+$ the group of rotation tensors, Sym and Skw the linear subspaces of symmetric and skew tensors and Sym^+ the positive-definite symmetric tensors; the symbol $\oplus$ is used to denote the direct sum of linear spaces. The tensor product of 3-vectors is indicated by interposing the symbol $\otimes$, and the Euclidean inner product of tensors $\mathbf{A}, \mathbf{B}$ is denoted by $\mathbf{A} \cdot \mathbf{B} = tr(\mathbf{A}\mathbf{B}^t)$; the associated norm is $|\mathbf{A}| = \sqrt{\mathbf{A} \cdot \mathbf{A}}$. In terms of orthogonal components, $\mathbf{A} \cdot \mathbf{B} = A_{ij}B_{ij}$, wherein the usual summation rule is implied. For a fourth-order tensor $\mathcal{A}$, the notation $\mathcal{A}[\mathbf{B}]$ stands for the second-order tensor with orthogonal components $\mathcal{A}_{ijkl}B_{kl}$. The transpose $\mathcal{A}^t$ is defined by $\mathbf{B} \cdot \mathcal{A}^t[\mathbf{A}] = \mathbf{A} \cdot \mathcal{A}[\mathbf{B}]$, and $\mathcal{A}$ is said to possess major symmetry if $\mathcal{A}^t = \mathcal{A}$. If $\mathbf{A} \cdot \mathcal{A}[\mathbf{B}] = \mathbf{A}^t \cdot \mathcal{A}[\mathbf{B}]$ and $\mathbf{A} \cdot \mathcal{A}[\mathbf{B}] = \mathbf{A} \cdot \mathcal{A}[\mathbf{B}^t]$ then $\mathcal{A}$ is said to possess minor symmetry. Finally, the notation $F_{\mathbf{A}}$ stands for the tensor-valued derivative of a scalar-valued function $F(\mathbf{A})$.

2. Basic theory

In the purely mechanical theory, variables of interest include the motion $\boldsymbol{\chi}(\mathbf{x},t)$ and the *plastic* deformation tensor $\mathbf{K}(\mathbf{x},t)$, where $\mathbf{x}$ is the position of a material point in a fixed reference placement κ_r of the body. The values $\mathbf{y}=\boldsymbol{\chi}(\mathbf{x},t)$ are the positions of these points at time t and generate the current placement κ_t of the body as $\mathbf{x}$ ranges over κ_r. The deformation gradient, $\mathbf{F}=\nabla\boldsymbol{\chi}$, is assumed to be invertible with $J_F>0$. These variables are used to define the *elastic* deformation

$$\mathbf{H}=\mathbf{F}\mathbf{K}. \tag{2}$$

We impose $J_H>0$ and conclude that $J_K>0$. The plastic deformation is related to the more commonly used measure $\mathbf{G}$ by $\mathbf{G}=\mathbf{K}^{-1}$.

The elastic strain energy of the body is

$$U=\int_{\kappa_t}\psi(\mathbf{H})dv, \tag{3}$$

where ψ is the spatial strain-energy density. Attention is confined to materially uniform bodies, exemplified by single crystals. These have the property that the strain-energy density does not depend explicitly on $\mathbf{x}$. However, most of the following discussion, concerned with local aspects of the theory, remains valid if this restriction is relaxed. We are concerned mainly with the constitutive structure of the theory and therefore restrict attention to smooth processes.

The local equations of motion are

$$div\mathbf{T}+\rho\mathbf{b}=\rho\ddot{\mathbf{y}},\quad \mathbf{T}\in Sym \quad \text{in} \quad \kappa_t, \tag{4}$$

where $\mathbf{T}$ is the Cauchy stress, ρ is the mass density, div is the spatial divergence (i.e., the divergence with respect to $\mathbf{y}$), superposed dots are used to denote material derivatives ($\partial/\partial t$ at fixed $\mathbf{x}$), and $\mathbf{b}$ is the body force per unit mass.

The decomposition (2) is associated with a vector space κ_i called the *local intermediate configuration*, which is mapped to the translation spaces of κ_r and κ_t by $\mathbf{K}$ and $\mathbf{H}$, respectively. Our main objective is to characterize intermediate configurations that are mechanically equivalent. To this end, several preliminary concepts are needed.

The strain-energy function referred to κ_i is

$$W(\mathbf{H})=J_H\psi(\mathbf{H}), \tag{5}$$

and generates the Cauchy stress via the formula [10]

$$\mathbf{T}\mathbf{H}^*=W_{\mathbf{H}}. \tag{6}$$

Necessary and sufficient for the symmetry of $\mathbf{T}$ (cf. $(4)_2$) is that W depend on $\mathbf{H}$ through the *elastic* Cauchy-Green deformation tensor [10]

$$\mathbf{C}=\mathbf{H}^t\mathbf{H}. \tag{7}$$

Thus,

$$W(\mathbf{H}) = \hat{W}(\mathbf{C}). \tag{8}$$

Equation (6) then provides

$$J_H \mathbf{T} = \mathbf{H}\mathbf{S}\mathbf{H}^t, \tag{9}$$

where $\mathbf{S}$ is the *elastic* 2nd Piola-Kirchhoff stress given by $\mathbf{S} = \hat{\mathbf{S}}(\mathbf{C})$, with

$$\hat{\mathbf{S}}(\mathbf{C}) = 2\hat{W}_{\mathbf{C}}. \tag{10}$$

It is usual to stipulate that κ_i is *undistorted*, or *natural*, in the sense that $\hat{\mathbf{S}}(\mathbf{I}) = \mathbf{0}$. Then, the strain-energy function W is subject to the restriction

$$W(\mathbf{H}) = W(\mathbf{H}\mathbf{R}), \tag{11}$$

where $\mathbf{R} \in Orth^+$ is an element of the symmetry group for the material (see [8,10] for further discussion). Using (10), it is straightforward to demonstrate that

$$\hat{\mathbf{S}}(\mathbf{R}^t\mathbf{C}\mathbf{R}) = \mathbf{R}^t\hat{\mathbf{S}}(\mathbf{C})\mathbf{R}. \tag{12}$$

To make use of restrictions arising from material symmetry in crystalline solids, it is necessary to specify information about the undistorted lattice (Section 5). It is shown in [10] that undistorted κ_i may be attained by an equilibrium (i.e., inertia-less) deformation of an arbitrarily small unloaded sub-body, granted the degree of smoothness required by the mean-stress theorem.

The sum of the kinetic and strain energies of an arbitrary part $p \in \kappa_t$ of the body is

$$\int_\pi \Phi dV; \quad \Phi = \Psi + \tfrac{1}{2}\rho_r \left|\dot{\mathbf{y}}\right|^2, \tag{13}$$

where π, with piecewise smooth boundary $\partial\pi$, is the region occupied by p in κ_r, and

$$\Psi(\mathbf{F}, \mathbf{K}) = J_K^{-1} W(\mathbf{F}\mathbf{K}) \tag{14}$$

is the referential strain-energy density.

The dissipation, $\mathcal{D}$, is the difference between the mechanical power P supplied to p and the rate of change of the total energy in p. Thus,

$$\mathcal{D} = P - \tfrac{d}{dt}\int_\pi \Phi dV. \tag{15}$$

This is expressible in the form [11]

$$\mathcal{D} = \int_\pi D dV, \tag{16}$$

where

$$D = \mathcal{E} \cdot \dot{\mathbf{K}}\mathbf{K}^{-1} \tag{17}$$

in which

$$\mathcal{E} = \Psi\mathbf{I} - \mathbf{F}^t\mathbf{P} \tag{18}$$

is Eshelby's energy-momentum tensor, and

$$\mathbf{P} = \mathbf{T}\mathbf{F}^* \tag{19}$$

is the usual Piola stress. Thus the dissipation is non-negative for every sub-body if and only if $D \geq 0$. We find it convenient to use (17) in the form

$$J_K D = \mathcal{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}}, \tag{20}$$

where

$$\mathcal{E}' = J_K \mathbf{K}^t \mathcal{E} \mathbf{K}^{-t} \tag{21}$$

is the Eshelby tensor, pushed forward to κ_i. This is purely elastic in origin. In particular [10],

$$\mathcal{E}'(\mathbf{C}) = \hat{W}(\mathbf{C})\mathbf{I} - \mathbf{C}\hat{\mathbf{S}}(\mathbf{C}), \tag{22}$$

implying that

$$\mathcal{E}'(\mathbf{R}^t\mathbf{C}\mathbf{R}) = \mathbf{R}^t\mathcal{E}'(\mathbf{C})\mathbf{R}, \tag{23}$$

if $\mathbf{R} \in Orth^+$ is a material symmetry transformation.

The equations of motion are augmented by a flow rule for the plastic deformation. Typically [10] this specifies $\mathbf{K}^{-1}\dot{\mathbf{K}}$ in terms of a constitutive response function, which must be such as to satisfy the material-symmetry transformation rule $\mathbf{K}^{-1}\dot{\mathbf{K}} \to \mathbf{R}^t(\mathbf{K}^{-1}\dot{\mathbf{K}})\mathbf{R}$. A framework for rate-independent response is described in Section 6.

3. Nilpotent plastic flows

Consider the linear space N of tensors with representative element $\mathbf{N}$ defined by

$$\mathbf{N} \cdot \mathcal{E}' = 0. \tag{24}$$

By writing

$$\mathcal{E}' = \mathbf{Z}\mathbf{C}^{-1} \quad \text{with} \quad \mathbf{Z}(\mathbf{C}) = \hat{W}(\mathbf{C})\mathbf{C} - \mathbf{C}\hat{\mathbf{S}}(\mathbf{C})\mathbf{C} \tag{25}$$

and invoking the symmetry of $\hat{\mathbf{S}}$, we have $\mathbf{Z}(\mathbf{C}) \in Sym$ and therefore

$$N \supseteq M = \{\mathbf{M}\colon\ \mathbf{M}\mathbf{C}^{-1} \in Skw\}, \tag{26}$$

in which $\mathbf{C}$ is associated with $\mathcal{E}'$ via (22).

M is the three-dimensional linear space spanned by $\{[Skw(\mathbf{e}_i \otimes \mathbf{e}_j)]\mathbf{C};\ i \neq j\}$, where $\{\mathbf{e}_i\}$ is any orthonormal basis for E^3. Its orthogonal complement with respect to Lin is

$$M^\perp = \{\mathbf{L}\colon\ \mathbf{L}\mathbf{C} \in Sym\}. \tag{27}$$

This is the six-dimensional linear space spanned by $\{[Sym(\mathbf{e}_i \otimes \mathbf{e}_j)]\mathbf{C}^{-1}\}$. Thus every tensor has a unique representation as the sum of elements of M and $M^\perp$. To establish that $N \subseteq M$, if true, and thus that $N = M$, we would need to show, given $\mathbf{C} \in Sym^+$, that $\mathbf{N} \cdot \mathcal{E}' = \mathbf{N}\mathbf{C}^{-1} \cdot \mathbf{Z}(\mathbf{C})$ vanishes only if $\mathbf{N}\mathbf{C}^{-1} \in Skw$. However, the premise does not preclude the possibility that $\mathbf{N}\mathbf{C}^{-1} \notin Skw$ because $\mathbf{Z}(\mathbf{C})$ is fixed by $\mathbf{C}$ and thus not an arbitrary element of Sym. If the elastic strain is small, as is often assumed in practice, then $\mathbf{C}$ may be replaced by $\mathbf{I}$ with an error on the order of the small strain, so that M is approximated by Skw.

It follows from the definitions that the projection of $\mathbf{K}^{-1}\dot{\mathbf{K}}$ onto M has no effect on dissipation. This leads us to pose the question of whether or not this projection plays an essential role, or if it can be suppressed without affecting the initial-boundary-value problem and hence without restricting the mechanical phenomena that the theory can be used to describe. This is more widely known as the problem of plastic spin, which has been a vexing issue in theories of plasticity that do not rely on slip-system kinematics. In the affirmative case the freedom afforded by the choice of κ_i may be used to simplify the theory accordingly. That this is possible in the case of isotropy has been firmly established in [2].

Indeed, if it is assumed that plastic flow is inherently dissipative [10]; i.e., that $D \geq 0$ and that D vanishes *if and only if* $\dot{\mathbf{K}}$ vanishes, then $\mathbf{K}^{-1}\dot{\mathbf{K}} \in M$ implies that $\dot{\mathbf{K}} = \mathbf{0}$. From this perspective elements of M do not qualify as *bona fide* plastic flows; we call them nilpotent flows. This is the content of the *principle of actual evolution* elucidated in [8]. This is not to say that the part of the plastic flow belonging to M *must* vanish, however. Here we study the role played by the projection of $\mathbf{K}^{-1}\dot{\mathbf{K}}$ onto M. In particular, we study the question of whether or not the restriction $\mathbf{K}^{-1}\dot{\mathbf{K}} \in M^{\perp}$ may be imposed without loss of generality. In the case of small elastic strain, this is equivalent to the question of whether or not the plastic spin may be suppressed.

4. Mechanical equivalence

Consider two local intermediate configurations, κ_{i_1} and κ_{i_2}, associated with a given reference placement κ_r. We wish to characterize the relationship between these configurations arising from the requirement that they be mechanically equivalent, in the sense that solutions to properly posed initial-boundary-value problems are invariant under replacement of one by the other. We begin by setting down some fairly obvious properties that one would expect of such a relationship.

(i) As a minimal requirement, we stipulate that mechanically-equivalent local intermediate configurations should correspond to the same motion $\mathbf{y} = \boldsymbol{\chi}(\mathbf{x}, t)$. They are therefore associated with one and the same deformation gradient $\mathbf{F}(\mathbf{x}, t)$. It follows from (2) that if $\mathbf{H}_1$ and $\mathbf{H}_2$ are the elastic deformations from κ_{i_1} and κ_{i_2} to κ_t, and if $\mathbf{K}_1^{-1}$ and $\mathbf{K}_2^{-1}$ are the plastic deformations from κ_r to κ_{i_1} and κ_{i_2}, then there is $\mathbf{A} \in Lin^+$ such that

$$\mathbf{H}_1 = \mathbf{H}_2\mathbf{A} \quad \text{and} \quad \mathbf{K}_1 = \mathbf{K}_2\mathbf{A}. \tag{28}$$

(ii) As further requirements, we impose the invariance of the Cauchy stress $\mathbf{T}(\mathbf{y}, t)$ and the strain energy stored in an arbitrary part of the body. Let $W_1(\mathbf{H}_1)$ and $W_2(\mathbf{H}_2)$ be the strain-energy functions associated with κ_{i_1} and κ_{i_2}. Then, from (6),

$$\mathbf{T}\mathbf{H}_1^* = (W_1)_{\mathbf{H}_1} \quad \text{and} \quad \mathbf{T}\mathbf{H}_2^* = (W_2)_{\mathbf{H}_2}. \tag{29}$$

Further, our assumptions imply that the referential strain energy density is invariant; eqs. (9), (14) then combine to yield

$$W_1(\mathbf{H}_1) = J_A W_2(\mathbf{H}_2) \quad \text{and} \quad J_A\mathbf{S}_2 = \mathbf{A}\mathbf{S}_1\mathbf{A}^t, \tag{30}$$

where $\mathbf{S}_{1,2}$ are the 2nd Piola-Kirchhoff stresses relative to $\kappa_{i_{1,2}}$, derived from W_1 and W_2 respectively by

formulas like (10). These relations ensure the mechanical equivalence of any pair of local configurations in the case of purely elastic response; i.e., in the absence of dissipation.

(iii) It is natural to impose the additional requirement that the dissipation be invariant for an arbitrary part of the body. Using (20) and $(28)_2$, the referential dissipation densities $D_{1,2}$ associated with $\kappa_{i_{1,2}}$ may be shown to satisfy

$$D_1 = D_2 + J_{K_2}^{-1}\mathcal{E}_2' \cdot \dot{\mathbf{A}}\mathbf{A}^{-1}, \tag{31}$$

where $\mathcal{E}_2'$ is the push-forward of the Eshelby tensor to κ_{i_2}, given by

$$\mathcal{E}_2' = \hat{W}_2\mathbf{I} - \mathbf{C}_2\mathbf{S}_2, \tag{32}$$

in which $\mathbf{C}_2 = \mathbf{H}_2^t\mathbf{H}_2$ and $\hat{W}_2(\mathbf{C}_2) = W_2(\mathbf{H}_2)$, use having been made of the connection

$$\mathcal{E}_1' = J_A\mathbf{A}^t(\mathcal{E}_2')\mathbf{A}^{-t}, \tag{33}$$

which follows from (21) and $(28)_2$.

The invariance of the dissipation; i.e., $D_1 = D_2$, is seen to follow if and only if

$$\mathcal{E}_2' \cdot \dot{\mathbf{A}}\mathbf{A}^{-1} = 0. \tag{34}$$

This may be recast as

$$(\mathbf{H}_2^t\mathbf{T}\mathbf{H}_2^* - W_2\mathbf{I}) \cdot \dot{\mathbf{A}}\mathbf{A}^{-1} = 0, \tag{35}$$

which in turn is equivalent, by virtue of $(28)_1$, to

$$\mathbf{T}\mathbf{H}_1^* \cdot \dot{\mathbf{H}}_1 = J_A\mathbf{T}\mathbf{H}_2^* \cdot \dot{\mathbf{H}}_2 + \dot{J}_A W_2, \quad \text{where} \quad \dot{J}_A = \mathbf{A}^* \cdot \dot{\mathbf{A}}. \tag{36}$$

Using (29) we find that this reduces to $\dot{W}_1 = (J_A W_2)^{\cdot}$, implying that W_1 is given, modulo an unimportant constant, by (30). It follows that (34) is necessary and sufficient for mechanical equivalence as stated thus far; namely, as the invariance of the deformation, the Cauchy stress, the energy (modulo a constant) and the dissipation.

Thus, with reference to (24) and (26), a transformation $\mathbf{A}(t) \in Lin^+$ that satisfies the differential equation

$$\dot{\mathbf{A}}\mathbf{A}^{-1} \in M_2 \tag{37}$$

where

$$M_\alpha = \{\mathbf{M}\colon\ \mathbf{M}\mathbf{C}_\alpha^{-1} \in Skw\}; \quad \alpha = 1, 2, \tag{38}$$

maps κ_{i_1} to a mechanically-equivalent κ_{i_2}.

We note that (37) yields a constant value of J_A. This follows easily from the vanishing of $\dot{J}_A/J_A = tr(\dot{\mathbf{A}}\mathbf{A}^{-1}) = tr(\mathbf{\Omega}_2\mathbf{C}_2)$, for any $\mathbf{\Omega}_2 \in Skw$. Therefore, solutions to (37) belong to Lin^+ if and only if $\mathbf{A}(t_0) \in Lin^+$. Given $\mathbf{A}(t_0)$, $\mathbf{A}(t)$ is uniquely determined by (37) for any - hence *every* - element of M_2. Further, every element of M_2 is expressible as $\dot{\mathbf{A}}\mathbf{A}^{-1}$ with $\mathbf{A}(t) \in Lin^+$.

From $(28)_2$ we have

$$\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 = \mathbf{A}^{-1}(\mathbf{K}_2^{-1}\dot{\mathbf{K}}_2 + \dot{\mathbf{A}}\mathbf{A}^{-1})\mathbf{A}. \tag{39}$$

We wish to know if it is possible to impose $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 \in M_1^\perp$ while preserving the mechanical equivalence of κ_{i_1} and κ_{i_2}. Thus we impose (37). We require the following simple lemma: Suppose $\mathbf{G}_1 \in M_1$ and define $\mathbf{G}_2$ by $\mathbf{A}^{-1}\mathbf{G}_2\mathbf{A} = \mathbf{G}_1$ for $\mathbf{A} \in Lin^+$. Then $\mathbf{G}_2 = \mathbf{A}\mathbf{\Omega}_1\mathbf{C}_1\mathbf{A}^{-1}$ for some $\mathbf{\Omega}_1 \in Skw$, and, from $(28)_1$, it follows that $\mathbf{G}_2 = \mathbf{A}\mathbf{\Omega}_1\mathbf{A}^t\mathbf{C}_2\mathbf{A}\mathbf{A}^{-1} = \mathbf{\Omega}_2\mathbf{C}_2$, where $\mathbf{\Omega}_2 = \mathbf{A}\mathbf{\Omega}_1\mathbf{A}^t \in Skw$. Therefore $\mathbf{G}_2 \in M_2$. We have shown that $M_2 = \mathbf{A}M_1\mathbf{A}^{-1}$; equivalently, $M_1 = \mathbf{A}^{-1}M_2\mathbf{A}$. Using this with (37), we conclude from (39), in which $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 \in M_1^\perp$ is imposed, that $\mathbf{A}^{-1}(\mathbf{K}_2^{-1}\dot{\mathbf{K}}_2)\mathbf{A} \in M_1 \oplus M_1^\perp = Lin$, which is equivalent to $\mathbf{K}_2^{-1}\dot{\mathbf{K}}_2 \in Lin$. Thus the restriction $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 \in M_1^\perp$ does not impose any restriction on $\mathbf{K}_2^{-1}\dot{\mathbf{K}}_2$.

In other words, given any plastic flow in Lin based on the use of κ_{i_2}, there exists a mechanically-equivalent κ_{i_1} such that $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 \in M_1^\perp$. This generalizes a result in [11] pertaining to small elastic strains. Because Lin is nine-dimensional whereas $M^\perp$ is only six-dimensional, it would thus appear that constitutive equations for plastic flow may be dramatically simplified without affecting the predictive capability of the theory. This is the point of view advanced in [11] for the case of small elastic strain. However, as argued in the next Section, this conclusion is premature.

5. Lattices

It is natural to appeal to concepts in crystal-elasticity theory in the course of contemplating further conditions to be imposed in a reasonable definition of mechanical equivalence for crystalline solids. Central to that theory is the idea that linearly independent lattice vectors $\mathbf{l}_i$ ($i \in \{1,2,3\}$) are mapped to their images $\mathbf{t}_i$ in κ_t in accordance with the Cauchy-Born hypothesis. To accommodate plasticity, this hypothesis is assumed to apply to the *elastic* deformation. Thus, $\mathbf{t}_t = \mathbf{H}\mathbf{l}_i$ where $\mathbf{l}_j$ are the lattice vectors in κ_i. It is natural to view the lattice set $\{\mathbf{l}_i\}$ associated with κ_i as an intrinsic property of the material. Accordingly, it is uniform (i.e., independent of $\mathbf{x}$) in a materially-uniform body.

The $\mathbf{t}_i$ are observable in principle. In practice they are computed from their measurable duals $\mathbf{t}^i$ [16]. We therefore extend the definition of mechanical equivalence to include the requirement that $\{\mathbf{t}_i\}$ be invariant. Further, (2) yields $\mathbf{t}_i = \mathbf{F}\mathbf{r}_i$, where $\mathbf{r}_i = \mathbf{K}\mathbf{l}_i$ are the lattice vectors in κ_r. Then, each $\mathbf{r}_i(= \mathbf{F}^{-1}\mathbf{t}_i)$ is also invariant, and

$$\mathbf{l}_{i(2)} = \mathbf{A}\mathbf{l}_{i(1)}; \quad \mathbf{A} = \mathbf{l}_{i(2)} \otimes \mathbf{l}^{i(1)}, \tag{40}$$

where $\mathbf{l}_{i(\alpha)}$, etc., are the lattice vectors in κ_{i_α}; $\alpha = 1,2$. A transformation from one local intermediate configuration to another mechanically equivalent one thus corresponds to a transformation of lattice vectors. The evolutions of these lattices are related by

$$\dot{\mathbf{l}}_{i(1)} = \mathbf{A}^{-1}[\dot{\mathbf{l}}_{i(2)} - \dot{\mathbf{A}}\mathbf{A}^{-1}\mathbf{l}_{i(2)}], \tag{41}$$

and they are mechanically equivalent if $\mathbf{A}(t)$ satisfies (37). Consequently the notion of mechanical equivalence may be phrased in terms of relationships among lattices associated with intermediate configurations. The plastic deformation is given by $\mathbf{K} = \mathbf{r}_i \otimes \mathbf{l}^i$, where the $\mathbf{l}^j$ are the duals of the $\mathbf{l}_j$. The elastic deformation is given by $\mathbf{H} = \mathbf{t}_i \otimes \mathbf{l}^i$; and the deformation gradient by $\mathbf{F} = \mathbf{t}_i \otimes \mathbf{r}^i$.

A trivial example of mechanical equivalence is furnished by the case $\mathbf{C}_2 = \mathbf{I}$. Then, (28) and (37) result in $\mathbf{A}(t) \in Orth^+$ and $\mathbf{C}_1 = \mathbf{I}$; the associated lattices are related by a rotation. If one is stress-

free, then both are stress-free by virtue of $(30)_2$. Therefore, undistorted lattices related by rotations are mechanically equivalent. If the elastic strain is small, then, to leading order, $\{\mathbf{l}_{i(2)}\}$ is related to a mechanically-equivalent $\{\mathbf{l}_{i(1)}\}$ by a rotation. In the case of finite elastic strain, the effect of a mechanically equivalent transformation is to induce a distortion of one lattice relative to the other. In this case a *rotation* generates a lattice that is *not* mechanically equivalent to the undistorted lattice.

When implementing the theory one encounters the need to specify the initial orientation of the lattice $\{\mathbf{l}_i\}$. This arises from the practical necessity to ensure that an initial value of the plastic deformation, and hence that of the stress via (2) and (9), can be fixed unambiguously, so that the initial-boundary-value problem consisting of the equation of motion and the flow rule for the plastic deformation can be forward-integrated in time. In the simplest case, guided by the natural view that the undistorted lattice is an intrinsic material property, the analyst would assume the $\mathbf{l}_i$ to be material vectors and thus impose $\dot{\mathbf{l}}_i = \mathbf{0}$, effectively fixing them once and for all. This is consistent with the notion that plasticity is associated with flow of material relative to the actual lattice, and the consequent fact that actual lattice vectors are not material vectors ($\dot{\mathbf{r}}_i \neq \mathbf{0}$ if and only if $\dot{\mathbf{K}} \neq \mathbf{0}$).

Having made this assumption, suppose the analyst uses κ_{i_2}, with $\dot{\mathbf{l}}_{i(2)} = \mathbf{0}$, together with some flow rule to compute a plastic flow $\mathbf{K}_2^{-1}\dot{\mathbf{K}}_2$. This flow may be used to construct $\mathbf{A}(t)$ in such a way as to eliminate the projection of $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1$, given by (39), onto M_1. Of course, the flow rule for $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1$ thus derived is automatically such that $\mathbf{K}_1^{-1}\dot{\mathbf{K}}_1 \in M_1^{\perp}$, and the associated lattice $\{\mathbf{l}_{i(1)}\}$, which is mechanically equivalent to $\{\mathbf{l}_{i(2)}\}$, satisfies $\dot{\mathbf{l}}_{i(1)} = -\mathbf{A}^{-1}\dot{\mathbf{A}}\mathbf{l}_{i(1)}$. Constitutive functions based on the use of $\{\mathbf{l}_{i(2)}\}$ may be used with the transformations (30) and (33) to compute their counterparts based on the evolving lattice $\{\mathbf{l}_{i(1)}\}$; these include a flow rule that is seemingly simplified by the fact that its projection onto M_1 vanishes. However, the computation of the lattice $\{\mathbf{l}_{i(1)}\}$ relative to which these apply requires the flow rule for κ_{i_2}, which may have a non-zero projection onto M_2. Said differently, to obtain the lattice relative to which plastic spin vanishes it is necessary to have knowledge of the plastic spin computed on the basis of the given lattice! Because of this there is no convincing basis for the belief, expressed by ourselves [10,11] and others, that plastic spin may be suppressed without loss of generality in flow rules for plastic evolution. On the contrary, the freedom to add M to $M^{\perp}$ in the formulation of flow rules may well be required to advance the theory to the point of offering meaningful agreement with empirical data. Nevertheless we show in the next Section that theory offers guidelines for narrowing the possibilities.

6. Example: rate-independent theory

Following conventional ideas for the description of rate-independent response we assume plastic flow to be possible only if the material is in a state of yield. We express this idea as the requirement that the elastic deformation belong to a manifold that may be parametrized by other variables. For example, motivated by G.I. Taylor's formula giving the flow stress as a function of dislocation density, and using the fact that the stress $\mathbf{S}$ may be expressed in terms of $\mathbf{C}$ via (10), we assume yield to be possible only

if [10,13]

$$G(\mathbf{C},\boldsymbol{\alpha})=0, \tag{42}$$

where G is a suitable yield function and

$$\boldsymbol{\alpha}=J_K\mathbf{K}^{-1}Curl\mathbf{K}^{-1} \tag{43}$$

is the (geometrically necessary) dislocation density. Here $Curl$ is the referential curl operation defined in terms of the usual vector operation by

$$(Curl\mathbf{A})\mathbf{c}=Curl(\mathbf{A}^t\mathbf{c}) \tag{44}$$

for any fixed vector $\mathbf{c}$. Relevant to our development is the *current* yield surface, defined, for fixed $\boldsymbol{\alpha}$, by $G(\cdot,\boldsymbol{\alpha})=0$. For simplicity's sake we assume G to be differentiable, so that the yield surface defines a differentiable manifold in Sym.

Plastic evolution; i.e., $\dot{\mathbf{K}}\neq\mathbf{0}$, is deemed to be possible only when (42) is satisfied, and the variable $\mathbf{C}$ is always constrained to belong to the *current elastic range* defined by $G(\cdot,\boldsymbol{\alpha})\leq 0$, assumed to be a connected set in Sym. In view of our restriction to materially uniform bodies we require that the same yield function pertain to all material points.

In [10] it is shown that (42) is invariant under superposed rigid-body motions and (global) changes of reference placement and is thus intrinsic to the material, provided that the *function* G is likewise invariant. Similar statements apply to the reduced strain-energy function (8) and to the associated stress, given by (10). In particular, the stated invariance properties are possessed by the tensors $\mathbf{C}$ and $\boldsymbol{\alpha}$ [10,17]. Further, the yield function is subject to the same material-symmetry restriction as that imposed on the strain-energy function; i.e. [10],

$$G(\mathbf{C},\boldsymbol{\alpha})=G(\mathbf{R}^t\mathbf{C}\mathbf{R},\mathbf{R}^t\boldsymbol{\alpha}\mathbf{R}). \tag{45}$$

It is important to note that the dislocation density is well-defined under symmetry transformations only if the symmetry group is discrete (see Theorem 8 of [7]). Accordingly, yield functions of the kind considered are meaningful only for crystalline solids.

The body is *dislocated* if $\boldsymbol{\alpha}$ does not vanish; in this case $\mathbf{K}^{-1}$ is not a gradient and from (2) it follows that neither is $\mathbf{H}$. In fact [17],

$$\boldsymbol{\alpha}=J_H\mathbf{H}^{-1}curl\mathbf{H}^{-1}, \tag{46}$$

in which $curl$ is the spatial curl. Then, κ_i has only local significance in the sense that it cannot be identified with a global placement of the body in Euclidean space. That is, a differentiable position field that identifies material points in κ_i does not exist.

Most workers assume the plastic evolution $\mathbf{K}^{-1}\dot{\mathbf{K}}$ to be such as to maximize the dissipation under the constraint that $\mathbf{C}$ belong to the current yield surface. This in turn is a provable consequence of the widely adopted I'llyushin postulate [18]. In the present context this condition takes the form [11]

$$[\mathcal{E}'(\mathbf{C})-\mathcal{E}'(\mathbf{C}^*)]\cdot\mathbf{K}^{-1}\dot{\mathbf{K}}\geq 0;\quad G(\mathbf{C},\boldsymbol{\alpha})=0, \tag{47}$$

where $\mathbf{C}^*$ is a fixed elastic strain in the elastic range. This inequality is preserved under material symmetry transformations. Thus the problem is to characterize the plastic flow such that the actual dissipation (cf. (20)) is maximized relative to that associated with any admissible elastic strain; i.e.,

$$\max(\mathcal{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}}) \quad \text{subject to} \quad G(\mathbf{C}, \boldsymbol{\alpha}) \leq 0, \tag{48}$$

which is a standard optimization problem with an inequality constraint. The Kuhn-Tucker necessary condition [19] immediately generates the flow rule

$$(\mathcal{E}'_{\mathbf{C}})^t[\mathbf{K}^{-1}\dot{\mathbf{K}}] = \mu G_{\mathbf{C}}, \tag{49}$$

where $\mu \in \mathbb{R}^+$ is a Lagrange multiplier and $(\mathcal{E}'_{\mathbf{C}})^t$, the transpose of the derivative of $\mathcal{E}'(\mathbf{C})$, is a linear transformation from Lin to Sym. If $\mu = 0$ then $\mathbf{K}^{-1}\dot{\mathbf{K}}$ belongs to the null space $\mathcal{N}$ of $(\mathcal{E}'_{\mathbf{C}})^t$. It follows from the fact that the domain and range of $(\mathcal{E}'_{\mathbf{C}})^t$ are respectively nine- and six-dimensional that $\mathcal{N}$ is necessarily three-dimensional.

Because of the role of the Eshelby tensor in inequality (47), and because the latter is so closely related to the elastic range, it is natural to consider yield functions that depend on $\mathbf{C}$ implicitly through $\mathcal{E}'$. This specialization is allowed by the invariance of the elastic range and the dissipation under superposed rigid-body motions and compatible changes of reference placement [10]. Thus we consider yield functions of the form

$$G(\mathbf{C}, \boldsymbol{\alpha}) = F(\mathcal{E}'(\mathbf{C}), \boldsymbol{\alpha}). \tag{50}$$

The elastic range is then the set $\mathcal{S}$ defined by $F(\mathcal{E}'(\cdot), \boldsymbol{\alpha}) \leq 0$, and we assume F to be differentiable. Further, F satisfies the material symmetry rule $F(\mathcal{E}', \boldsymbol{\alpha}) = F(\mathbf{R}^t\mathcal{E}'\mathbf{R}, \mathbf{R}^t\boldsymbol{\alpha}\mathbf{R})$.

Of course $\mathcal{E}'(\mathbf{C}) \in Lin$ for every $\mathbf{C} \in Sym^+$, but in general not every element of Lin is expressible in the form $\mathcal{E}'(\mathbf{C})$; that is, there is not a unique element of Sym^+ corresponding to a given element of Lin. This issue is central to the considerations of [14,15]. Following that work we define a second elastic range $\mathcal{K}$ by the requirement $F(\cdot, \boldsymbol{\alpha}) \leq 0$ in which the domain is now Lin. It is then clear that $\mathcal{S} \subset \mathcal{K}$. We also have $\mathcal{S} \subseteq \mathcal{T} \subset \mathcal{K}$, where $\mathcal{T} = \mathcal{K} \cap \mathcal{M}$ and $\mathcal{M}$ is the subset of Lin defined by $\mathcal{E}'\mathbf{C} \in Sym$. However, we cannot assert that $\mathcal{S}$ and $\mathcal{T}$ are equivalent unless we can show that the equation

$$\mathcal{E}'\mathbf{C} = \hat{W}(\mathbf{C})\mathbf{C} - \mathbf{C}\hat{\mathbf{S}}(\mathbf{C})\mathbf{C} \tag{51}$$

has a unique solution $\mathbf{C} \in Sym^+$ for every $\mathcal{E}' \in \mathcal{M}$. That is, the restriction $\mathcal{E}'\mathbf{C} \in Sym$ for $\mathcal{E}' \in Lin$ and $\mathbf{C} \in Sym^+$ does not in general yield a unique $\mathbf{C}$ such that $\mathcal{E}' = \mathcal{E}'(\mathbf{C})$. Having said this we note that if the elastic strain is small, then (51) reduces to $\mathbf{S} = -Sym\mathcal{E}'$ to leading order, which has a unique solution for the elastic strain $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$ under realistic hypotheses on the elastic constitutive response [10,11]. This yields a unique $\mathbf{C} \in Sym^+$ provided that $|Sym\mathcal{E}'|$ is not too large. Thus, as a practical matter, we expect $\mathcal{S}$ and $\mathcal{T}$ to be equivalent in real metallic crystals in which the elastic strain is invariably small. In connection with this point we remark that a counter-example has been exhibited in [14] showing that in general no bijection exists between $\mathcal{S}$ and $\mathcal{K}$. However, this demonstration makes use of extreme elastic strains that undoubtedly lie well outside the elastic range of any real metallic crystal and, as such, are physically inadmissible. This observation lends further support to the plausibility of our assumption that $\mathcal{S}$ and $\mathcal{T}$ are equivalent in practical applications.

The foregoing inclusions suggest that we replace (48) by the problem

$$\max(\mathcal{E}' \cdot \mathbf{K}^{-1}\dot{\mathbf{K}}) \quad \text{subject to} \quad F(\mathcal{E}', \boldsymbol{\alpha}) \leq 0 \quad \text{and} \quad \mathbf{W} = \mathbf{0}, \tag{52}$$

where

$$\mathbf{W} = Skw(\mathcal{E}'\mathbf{C}). \tag{53}$$

The constraints are equivalent to the requirement $\mathcal{E}' \in \mathcal{T}$, whereas $F(\cdot, \boldsymbol{\alpha})$ is defined on Lin. Thus we regard $F(\cdot, \boldsymbol{\alpha})$ as a smooth extension of $F(\mathcal{E}'(\cdot), \boldsymbol{\alpha})$ from $\mathcal{T}$ to Lin and satisfying the same material symmetry rule. We now have an optimization problem with both inequality and equality constraints. The relevant version of the Kuhn-Tucker necessary condition for this problem is [19]

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = (\lambda F + \boldsymbol{\Omega} \cdot \mathbf{W})_{\mathcal{E}'}, \tag{54}$$

where $\lambda \in \mathbb{R}^+$ and $\boldsymbol{\Omega} \in Skw$ are Lagrange multipliers and the derivative $F_{\mathcal{E}'}$, an element of Lin, is evaluated on $\mathcal{T}$. It is straightforward to derive $(\boldsymbol{\Omega} \cdot \mathbf{W})_{\mathcal{E}'} = \boldsymbol{\Omega}\mathbf{C}$ and thus to obtain the flow rule

$$\mathbf{K}^{-1}\dot{\mathbf{K}} = \lambda F_{\mathcal{E}'} + \boldsymbol{\Omega}\mathbf{C}. \tag{55}$$

We observe from (26) that the term $\boldsymbol{\Omega}\mathbf{C}$ belongs to the three-dimensional space M and is therefore nilpotent. Therefore the dissipation is (cf. (20))

$$J_K D = \lambda \mathcal{E}' \cdot F_{\mathcal{E}'}. \tag{56}$$

Because $\lambda \geq 0$, the dissipation is positive only if $\lambda > 0$ and thus only if $\mathcal{E}' \cdot F_{\mathcal{E}'} > 0$. Further, material symmetry transformations yield $F_{\mathcal{E}'} \to \mathbf{R}^t F_{\mathcal{E}'} \mathbf{R}$ and (55) then requires that $\boldsymbol{\Omega} \to \mathbf{R}^t \boldsymbol{\Omega} \mathbf{R}$.

In [10] a constitutive hypothesis is made to the effect that contributions to the flow rule of the form $\boldsymbol{\Omega}\mathbf{C}$ may be suppressed. While this is permissible from the viewpoint of mechanical equivalence as defined in Section 4, it is restrictive from the viewpoint discussed in Section 5. Nevertheless it is possible to derive certain restrictions that $\boldsymbol{\Omega}$ must satisfy.

To this end we use the chain rule on $\mathcal{S}$ (assumed equivalent to $\mathcal{T}$), obtaining

$$G_{\mathbf{C}} = (\mathcal{E}'_{\mathbf{C}})^t [F_{\mathcal{E}'}]. \tag{57}$$

Comparison of (49) and (55) shows that the combination $(\lambda - \mu)F_{\mathcal{E}'} + \boldsymbol{\Omega}\mathbf{C}$ belongs to the null space $\mathcal{N}$ of $(\mathcal{E}'_{\mathbf{C}})^t$. However, this is possible only if $\mu = \lambda$ because $F_{\mathcal{E}'} \in Lin$ whereas $\mathcal{N}$ is three dimensional. Indeed, at this stage λ and μ are arbitrary non-negative scalars and the imposition of $\mu = \lambda$ in (49) and (55) entails no loss of generality. Consequently $\boldsymbol{\Omega}$ is restricted by the requirement $\boldsymbol{\Omega}\mathbf{C} \in \mathcal{N}$; i.e.,

$$(\mathcal{E}'_{\mathbf{C}})^t [\boldsymbol{\Omega}\mathbf{C}] = \mathbf{0}. \tag{58}$$

This result is more stringent than that derived in [14,15]. In that work the extension of the Kuhn-Tucker theorem to equality- and inequality-constrained problems is not used and attention is confined to the case of plastic incompressibility. In terms of the present model it is shown there that $\mathbf{K}^{-1}\dot{\mathbf{K}} - \lambda F_{\mathcal{E}'} \in \mathcal{N}$. Here we have $\mathbf{K}^{-1}\dot{\mathbf{K}} - \lambda F_{\mathcal{E}'} \in M \cap \mathcal{N}$, which simplifies the problem of deriving restrictions on $\boldsymbol{\Omega}$.

To make the problem (58) explicit we need to characterize the null space $\mathcal{N}$. Thus consider a one-parameter family of elastic deformations $\mathbf{C}(u) \in Sym^+$ with u in some open interval. Differentiating (22) with respect to u furnishes

$$\mathcal{E}'_{\mathbf{C}}[\dot{\mathbf{C}}] = \dot{W}\mathbf{I} - \dot{\mathbf{C}}\mathbf{S} - \mathbf{C}\dot{\mathbf{S}}. \tag{59}$$

Using (10) in the form $\dot{W} = \frac{1}{2}\hat{\mathbf{S}} \cdot \dot{\mathbf{C}}$ and $\dot{\mathbf{S}} = 2\hat{W}_{\mathbf{CC}}[\dot{\mathbf{C}}]$ and noting that $\dot{\mathbf{C}} \in Sym$ may be chosen arbitrarily, we derive

$$\mathcal{E}'_{\mathbf{C}}[\mathbf{B}] = \tfrac{1}{2}(\hat{\mathbf{S}} \cdot \mathbf{B})\mathbf{I} - \mathbf{B}\hat{\mathbf{S}} - 2\mathbf{C}(\hat{W}_{\mathbf{CC}}[\mathbf{B}]) \quad \text{for all} \quad \mathbf{B} \in Sym. \tag{60}$$

Thus for any $\mathbf{A} \in Lin$,

$$\mathbf{B} \cdot (\mathcal{E}'_{\mathbf{C}})^t[\mathbf{A}] = \mathbf{A} \cdot \mathcal{E}'_{\mathbf{C}}[\mathbf{B}] = \tfrac{1}{2}(\hat{\mathbf{S}} \cdot \mathbf{B})\mathbf{I} \cdot \mathbf{A} - \mathbf{A} \cdot \mathbf{B}\hat{\mathbf{S}} - 2\mathbf{A} \cdot \mathbf{C}(\hat{W}_{\mathbf{CC}}[\mathbf{B}]). \tag{61}$$

Using the properties of the inner product, the symmetry of $\hat{\mathbf{S}}$ and the major symmetry of $\hat{W}_{\mathbf{CC}}$, we recast this as

$$\mathbf{B} \cdot (\mathcal{E}'_{\mathbf{C}})^t[\mathbf{A}] = \tfrac{1}{2}(\mathbf{I} \cdot \mathbf{A})\mathbf{B} \cdot \hat{\mathbf{S}} - \mathbf{B} \cdot Sym(\mathbf{A}\hat{\mathbf{S}}) - 2\mathbf{B} \cdot \hat{W}_{\mathbf{CC}}[\mathbf{A}^t\mathbf{C}]. \tag{62}$$

Accordingly, because $\mathbf{B}$ is an arbitrary element of Sym,

$$(\mathcal{E}'_{\mathbf{C}})^t[\mathbf{A}] = \tfrac{1}{2}(\mathbf{I} \cdot \mathbf{A})\hat{\mathbf{S}} - Sym(\mathbf{A}\hat{\mathbf{S}}) - 2\hat{W}_{\mathbf{CC}}[\mathbf{A}^t\mathbf{C}] \quad \text{for all} \quad \mathbf{A} \in Lin, \tag{63}$$

and $\mathcal{N}$ is the set of all tensors that annul the right-hand side. It is straightforward to show that the material symmetry $\mathcal{N} \to \mathbf{R}^t\mathcal{N}\mathbf{R}$ is satisfied (see also [14]).

For $\mathbf{A} = \mathbf{\Omega}\mathbf{C}$ with $\mathbf{\Omega} \in Skw$ we have $\mathbf{I} \cdot \mathbf{A} = tr(\mathbf{\Omega}\mathbf{C}) = \mathbf{\Omega} \cdot \mathbf{C}$, which vanishes identically. Further, $\mathbf{A}^t\mathbf{C} = -\mathbf{C}\mathbf{\Omega}\mathbf{C} \in Skw$, and $\hat{W}_{\mathbf{CC}}[\mathbf{A}^t\mathbf{C}]$ thus vanishes by the minor symmetry of $\hat{W}_{\mathbf{CC}}$. Therefore (58) reduces to

$$Sym[\mathbf{\Omega}\mathbf{C}\hat{\mathbf{S}}(\mathbf{C})] = \mathbf{0}, \tag{64}$$

which is equivalent to

$$Sym[\mathbf{\Omega}\mathcal{E}'(\mathbf{C})] = \mathbf{0} \tag{65}$$

by virtue of (22). These restrictions are preserved under material symmetry transformations $\mathbf{R} \in Orth^+$. We emphasize the fact (64) is not a general requirement. It applies only in the case of yield functions that depend on $\mathbf{C}$ via $\mathcal{E}'(\mathbf{C})$, and even then only when the restrictions described in the paragraph containing (51) are satisfied.

For small elastic strain $\mathbf{C}\hat{\mathbf{S}}(\mathbf{C})$ is of order $|\mathbf{E}|$ where $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$. This vanishes at leading order; i.e., at order unity, reducing (64) to an identity. In this case there are no *a priori* restrictions on $\mathbf{\Omega}$ apart from the requirement that its constitutive specification satisfy material symmetry. In the general case (64) (or (65)) connects $\mathbf{\Omega}$ to the elastic deformation and to the crystal properties via the stress-deformation relation. The characterization of solutions $\mathbf{\Omega}$ thus requires detailed consideration of the particular crystalline response at hand.

It is appropriate to regard (2) and the equations of motion (4), together with the elastic constitutive equation (9), the yield function and the flow rule, as constituting an initial-boundary-value problem for the deformation $\boldsymbol{\chi}(\mathbf{x}, t)$ and plastic deformation $\mathbf{K}(\mathbf{x}, t)$. In particular, the flow rule requires the

specification of an initial value $\mathbf{K}_0(\mathbf{x}) = \mathbf{K}(\mathbf{x}, t_0)$. Granted $\{\mathbf{l}_i\}$, this is given via $\mathbf{K}_0(\mathbf{x}) = \mathbf{r}_i(\mathbf{x},t_0) \otimes \mathbf{l}^i$ by the values of the referential lattice vectors $\mathbf{r}_i(\mathbf{x},t_0) = \mathbf{F}(\mathbf{x}, t_0)^{-1}\mathbf{t}_i(\mathbf{x}, t_0)$, wherein $\mathbf{t}_i$ are computed from their empirically determined duals $\mathbf{t}^i$ [16]. The latter are then predicted at any time $t_1 > t_0$ by the coupled theory for the fields $\boldsymbol{\chi}$ and $\mathbf{K}$, and constitutive equations for $\boldsymbol{\Omega}$, subject to (64), may be adjusted as needed to enhance agreement with the measured field $\mathbf{t}^i(\mathbf{x}, t_1)$. To be sure this is a formidable task, but one which is ultimately necessary for the assessment of the predictive potential of any theory for plastic flow in crystalline solids.

Acknowledgment: DJS thanks John Edmiston of UC Berkeley for helpful discussions on the subject of plastic slip.

References

1. K.S. Havner, 1992, *Finite Plastic Deformation of Crystalline Solids.* Cambridge University Press.

2. M.E. Gurtin, E. Fried and L. Anand, 2010, *Mechanics and Thermodynamics of Continua.* Cambridge University Press.

3. S. Ha and K. T. Kim, 2011, Heterogeneous deformation of Al single crystal: Experiments and finite element analysis. Math. Mech. Solids 16, 652-661.

4. V.A. Lubarda, 2002, *Elastoplasticity Theory.* CRC Press, Boca Raton, FL.

5. G. Rengarajan and K. Rajagopal, 2001, On the form for the plastic velocity gradient L_p in crystal plasticity. Math. Mech. Solids 6, 471-80.

6. L. Deseri and D.R. Owen, 2002, Invertible structured deformations and the geometry of multiple slip in single crystals. Int. J. Plasticity 18, 833-849.

7. W. Noll, 1967, Materially uniform simple bodies with inhomogeneities. Arch. Ration. Mech. Anal. 27, 1-32.

8. M. Epstein and M. Elzanowski, 2007, *Material Inhomogeneities and their Evolution.* Springer, Berlin.

9. S. Cleja-Tigoiu and E. Soos, 1990, Elastoviscoplastic models with relaxed configurations and internal variables. Appl. Mech. Reviews 43, 131-51.

10. A. Gupta, D.J. Steigmann and J.S. Stölken, 2007, On the evolution of plasticity and incompatibility. Math. Mech. Solids 12, 583-610.

11. A. Gupta, D.J. Steigmann and J.S. Stölken, 2011, Aspects of the phenomenological theory of elastic-plastic deformation. J. Elasticity 104, 249-266.

12. J. Lubliner, 1986, Normality rules in large-deformation plasticity. Mechanics of Materials 5, 29-34.

13. J. Lubliner, 2008, *Plasticity Theory.* Dover, New York.

14. S. Cleja-Tigiou, 2003, Consequences of the dissipative restrictions in finite anisotropic elastoplasticity. Int. J. Plasticity 19, 1917-1964.

15. S. Cleja-Tigoiu, 2003, Dissipative nature of plastic deformations in finite anisotropic elasto-

plasticity. Math. Mech. Solids 8, 575-613.

16. B. Cullity, 1978, *Elements of X-Ray Diffraction.* Addison-Wesley.

17. P. Cermelli and M.E. Gurtin, 2001, On the characterization of geometrically necessary dislocations in finite plasticity. J. Mech. Phys. Solids 49, 1539-68.

18. M. Lucchesi and M. Silhavy, 1991, Il'yushin's conditions in non-isothermal plasticity. Arch. Ration. Mech. Anal. 113, 121-63.

19. W.I. Zangwill, 1969, *Nonlinear Programming.* Prentice-Hall, Englewood Cliffs, N.J.