Plasticity and non-Schmid effects

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The structure of the overall response of a metal polycrystal is analysed under the assumption that activity on the slip systems of its constituents is governed by a generalized Schmid law. In the resulting macromodel of metal plasticity, the overall rate of plastic deformation is related to the stress gradient of the yield surface via a generalized, but still associated, flow rule. While the overall rate of plastic deformation is no longer collinear with the stress gradient of the yield surface, its deviation is characterized by an additional macrovariable, representative of the rate of the non-Schmid effects taking place at constituent level.

1. Introduction

The basic phenomenology of crystal plasticity was clarified in the early 1900s when it was recognized that crystals deform by plastic shearing along crystallographic directions [1,2]; see also the brief but very informative introduction into the early history of crystal plasticity in Asaro [3]. At about the same time, it was also proposed, and later confirmed by direct observations, that plastic shear is, in fact, the result of the motion of numerous dislocations (one-dimensional crystal defects) along crystallographic planes and directions, a process called slip. The specific crystallographic planes and directions along which a crystal can be deformed by plastic shearing are called slip systems. The Schmid law is the constitutive link between the crystal kinematics and the stress field generated within the crystal by external loading. It states that shearing on a slip system can be initiated only if its corresponding resolved shear stress reaches a critical value [4]. When all slip systems are considered, the Schmid law defines a yielding (or activation) surface in stress space and, in the rigid–plastic approximation, the rate of deformation lies within the normal cone at the current stress state on the yielding surface. When aggregates of many
crystals are considered and the Taylor [2] homogenization principle is employed (each constituent experiences the deformation imposed at the boundary of the aggregate), this geometrical structure propagates virtually intact at macrolevel: the macrorate of deformation is along the exterior normal to the overall yield surface [5,6].

The theory was later extended to allow for arbitrary elastic strains [7,8], and for general conditions for estimating the overall response of an aggregate [9]. However, in the elastic–plastic context, the normality structure of the theory does not seem to be quite so straightforward: in Rice [7, p. 433] it was conditioned by the assumption that ‘the rate of progression of any local micro-structural rearrangement within the material is dependent on the current stress state only through the thermodynamic force conjugate to the extent of that rearrangement’; in Hill & Rice [8], it was recognized that normality depends on the evolution law assigned to the slip systems of a constituent. The matter is reconsidered in Soare [10] where the structure of the macroscopic constitutive model is deduced for a quite general class of slip system evolutions; in particular, if the slip systems convect with the lattice of a constituent, then the macromodel enjoys the normality structure.

On the other hand, phenomena such as cross-slip of dislocations [11], pressure dependence of yielding [12] or effects of non-glide stresses on slip system yielding in intermetallic alloys [13], imply that the Schmid law may provide only an approximate description of the forces governing slip activity; hence, the normality rule may also provide just an approximate description of the direction of plastic flow. The question is then: what is the precise relationship, if any, between the direction of plastic flow and the yield surface, at both single-crystal and macro levels when generalizations of Schmid activation criterion are considered? It appears that the question is not trivial, since violations of the Schmid law (or non-Schmid effects) at the crystal level have been usually interpreted as an indication that in continuum models of metal plasticity, the yield surface no longer determines the direction of plastic flow, via the normality rule, and that an additional constitutive element, in the form of a plastic potential, would be required to characterize the direction of plastic flow [14,15].

Here, we consider a polycrystal aggregate for which a generalized Schmid law controls slip at constituent level, and aim at deducing the structure of the overall response of the aggregate. The approach is similar to that in Soare [10] but the framework is different. Since the symmetry of the instantaneous elastic moduli is crucial for both theoretical and practical considerations, and with an eye to further applications, the constitutive response of a constituent will be explicitly hyperelastic. A general theory of the elastic–plastic response of such aggregates has been described by Hill & Rice [16]. Most of the present developments will be featured in the context of this theory. At its foundations lies the parametrization of the plastic state; while in the cited work, this is left at an abstract level, the aim being at a general theory, here the multiplicative elastic–plastic decomposition of Rice [7] is used explicitly to construct parametrizations of the plastic state at crystal level.

2. Single-crystal model: basic equations

We begin our analysis from what is actually observed. Thus, we write the basic equations characterizing the response of a crystal by first referring them to a spatial (or laboratory) frame (Eulerian description). Then, considering a crystal deformed plastically by shearing along crystallographic directions, an observer of the resulting motion writes [8,11,17]

\[
d = d^e + \dot{d}^p, \quad w = w^e + w^p, \quad \dot{P}^e := \dot{d}^p + w^p, \quad \dot{\tau}^e := \dot{\tau}^e + \dot{\tau}^p,
\]

(2.1)

\[
\dot{d}^p := \sum_{\alpha \in A} \dot{\gamma}^a \alpha^\alpha, \quad w^p := \sum_{\alpha \in A} \dot{\gamma}^a \alpha^a
\]

(2.2)

and

\[
\dot{\tau}^e := \dot{\tau} + \tau w^e - w^e \tau = K^e : (d - \dot{d}^p),
\]

(2.3)
where \( I = d + w \) represents the decomposition of the spatial gradient \( I \) of the local velocity field into the rate of deformation and spin, \( A \) denotes the set of active slip systems at a material point of the crystal, \( \gamma^\alpha \) denotes the rate of plastic shear on the slip system \( \alpha \),

\[
\alpha^\alpha := \frac{1}{2}(m^\alpha \otimes n^\alpha + n^\alpha \otimes m^\alpha) \quad \text{and} \quad b^\alpha := \frac{1}{2}(m^\alpha \otimes n^\alpha - n^\alpha \otimes m^\alpha).
\]

\( \{m^\alpha, n^\alpha\} \) and \( \{-m^\alpha, n^\alpha\} \) are viewed as two distinct slip systems; hence \( \gamma^\alpha > 0 \), for all \( \alpha \in A \).

\( K^l \) is the tensor of instantaneous elastic moduli associated with the Jaumann rate of the Kirchhoff stress \( \tau := J\sigma \), where \( J \) is the determinant of the deformation gradient (with respect to some reference configuration) and \( \sigma \) is the Cauchy stress. Equation (2.3) reproduces the point of view of an observer attached to a frame spinning at the rate \( w^\alpha \), the spin of the crystal lattice with respect to the material. The point of view of an observer attached to a frame spinning with the material is obtained by rearranging equation (2.3) in the form

\[
\tau^l := \dot{\tau} + \tau w - w\tau = K^l : (d - d^p),
\]

where

\[
d^p := \tilde{d}^p - (K^l)^{-1} : (\tau w^p - w^p\tau).
\]

Of further interest is the restatement of the above stress–strain relationship in terms of the Truesdell stress rate. A rearrangement of equation (2.5) yields

\[
\tau^l := \dot{\tau} - l\tau - \tau\dot{l} = K^l : (d - d^{pl}),
\]

where, based on the relationship \( \tau^l = \dot{\tau} - (\tau d + d\tau) \), for any symmetric second-order tensor \( d^\alpha \), the tensor of instantaneous moduli \( K^l \) is defined by \( K^l : d^\alpha := K^l : d^\alpha - (\tau d\tau + d^\alpha\tau) \). The corresponding rate of plastic deformation, as measured by an observer attached to a Truesdell frame (i.e. a frame convecting with the motion), is

\[
d^{pl} := (K^{l*})^{-1} K^l : d^\alpha = \tilde{d}^p + (K^l)^{-1} : (\tau P^T + P^T\tau).
\]

3. Single-crystal model with elastic potential

Defining an elastic potential requires a parametrization of the plastic state. It seems that the most convenient way to achieve this is by using the multiplicative elastic–plastic decomposition of the deformation gradient with respect to a reference configuration.

Then, let \( B_0 \subset R^3 \) denote a reference configuration of a crystal subjected to the motion \( x = \hat{x}(X, t), X \in B_0, t \in [0, \infty) \). The motion, \( B_0 \), and the current configuration \( B_t := (\hat{x}(X, t))X \in B_0 \) of the crystal are referred to a common Cartesian (fixed) frame. At each material particle \( X \), a multiplicative decomposition of the deformation gradient \( F(X) \) is assumed to exist [7],

\[
\frac{\partial \hat{x}}{\partial X}(X, t) := F(X, t) = F^p(X, t)F^p(X, t).
\]

Thinking of the crystal as a composite consisting of ‘material’ and ‘lattice’, \( F^p \) is to represent the plastic shearing of material (through the crystal lattice) and \( F^p \) is the accompanying elastic distortion during which the lattice and material deform as one; see Asaro & Rice [11] or Asaro [17] for a pictorial representation. \( F^p \) also incorporates the local rotation of the crystal owing to the constraints imposed by the neighbouring material (through boundary conditions). In general, the decomposition (3.1) is not expected to be compatible, in the sense that, in general, \( F^p \) and \( F^p \) may not be the gradients of some smooth motions. If \( T_X \) and \( T_x \) denote, respectively, the tangent spaces at the reference and current configurations at particle \( X \) and its position \( x = \hat{x}(X, t) \), then the collection \( B^p := \{F^p : T_X \rightarrow T_x \mid X \in B_0\} \) is usually referred to as the intermediate configuration\(^1\) of the crystal. Here, the term ‘configuration’ is used loosely because \( B^p \) is not a (differentiable) manifold in the Euclidean ambient space of the motion \( \hat{x} \) [18,19].

\(^1\)Current practice defines this as the set \( B^p := \{F^p : T_X \rightarrow T_x \mid X \in B_0\} \) with \( T_x^p \) linear spaces associated with the intermediate configuration; however, since plastic deformation does not affect the lattice, one can make the identification \( T_X^p \approx T_X \).
Taking the time rate in equation (3.1), with \( I := \dot{F}^{-1}, I^* := \dot{F}^* F^{-1} \) and \( L^p := \dot{F}^p F^{-1} \), one obtains
\[
I = I^* + F^* L^p F^* - 1. \tag{3.2}
\]
In particular, if the reference configuration is the current configuration, then the above additive decomposition of \( I \) must be identical with the decomposition \( I = I^* + \dot{F}^p \) featured in equations (2.1) and (2.2), since the two decompositions are supposed to describe the same kinematics. Furthermore, this must hold for any reference configuration and so \( F^* L^p F^* - 1 = \dot{F}^p = \sum_{\alpha \in A} \dot{\gamma}^\alpha m^\alpha \otimes n^\alpha, \) which is equivalent to \( L^p = \sum_{\alpha \in A} \dot{\gamma}^\alpha (F^* - 1 : m^\alpha) \otimes (F^*T : n^\alpha). \) Then, given \( m^\alpha \) and \( n^\alpha \) unit vectors in the slip and normal directions in the reference configuration \( B_0, \) the following (natural) evolution law is adopted for the slip systems of the crystal:
\[
m^\alpha = F^* : m^\alpha \quad \text{and} \quad n^\alpha = F^{*-T} : n^\alpha \implies L^p = \sum_{\alpha \in A} \dot{\gamma}^\alpha G^\alpha,
\]
where
\[
G^\alpha := m^\alpha \otimes n^\alpha.
\]
Thus, \( \{m^\alpha, n^\alpha\} \) convect with the lattice, and an observer placed in a frame convecting with the lattice will measure plastic strain as if this would take place in an undistorted (reference) crystal.

There are many other plausible evolution laws that could be assigned to the slip systems [8,11]. In the context of decomposition (3.2), once such an evolution law is assigned to the slip systems, then the corresponding characterization of \( L^p \) follows. For example, if the slip systems are assumed to just rotate rigidly at the spin of the lattice, a case investigated in Soare [10], i.e. \( \dot{m}^\alpha = w^*: m^\alpha \) and \( \dot{n}^\alpha = w^*: n^\alpha, \) with \( w^* := (I^* - I^T)/2, \) then one can show that \( L^p = \sum_{\alpha \in A} \dot{\gamma}^\alpha U^{*^{-1}}R_{u^*}^T G^\alpha R_{u^*T} U^* \), where \( F^* = R_u U^* \) is the polar decomposition of \( F^* \) and \( R_u^* \) is the rotation at spin \((U^* U^{*^{-1}} - U^{u*^{-1}} U^*)/2. \) Throughout the rest of this work, it will be assumed that the slip systems evolve according to equation (3.3). The main consequence of this assumption is that, in the absence of non-Schmid effects, the structure of the constitutive system at micro- and macrolevels enjoys the normality structure [8,10].

As stress and strain measures on \( B_0, \) we adopt the conjugate pair of the symmetric Kirchhoff stress and Green strain, that is, \( S := F^{-1} (\sigma) F^T \) and \( E := (F^T F - I)/2. \) Although the next arguments extend to other stress–strain measures [20], formulae and derivations are the simplest when the pair \((S, E)\) is used. The reason for this is that simple and explicit pullback/pushforward formulae relate \((S, E)\) to \((\sigma, d\ell), \) for any reference configuration, where the fundamental formula \( D := E = F^T dF \) is recalled. The same pullback formula must hold for the rate \( \dot{D}^p \) defined in equations (2.1) and (2.2), and hence its image in the reference configuration is
\[
\dot{D}^p := F^T \dot{F}^p F = \sum_{\alpha \in A} \gamma^\alpha A^\alpha, \tag{3.4}
\]
with
\[
A^\alpha := F^T a^\alpha F = F^T F^{-1}/2 (C^* G^\alpha + G^\alpha T C^*) F^p,
\]
where \( C^* := F^T F^*. \) With \( K^L \) now defined by \( K^L := a = F [K : (F^T aF)] F^T, \) for any second-order symmetric tensor \( a, \dot{D}^{pl} := F^T \dot{d}^{pl} F \) then acquires the following representation:
\[
\dot{D}^{pl} = \dot{D}^p + K^{-1} : (S \dot{F}^T L^p F^p - T + F^p^{-1} L^p F^p S)
= \sum_{\alpha \in A} \gamma^\alpha [A^\alpha + K^{-1} : (SH^\alpha T + H^\alpha S)], \tag{3.5}
\]
obtained by using equations (2.8) and (3.3), and where
\[
H^\alpha := F^p^{-1} G^\alpha F^p. \tag{3.6}
\]
The as-yet unspecified Lagrangian tensor of elasticity \( K \) is now defined by assuming the crystal enjoys a hyperelastic response. The safest approach to defining the latter is via the theory of elastic–plastic deformation developed by Hill & Rice [16]. Here, as a particularization of this theory, it is assumed that there exists a symmetric second-order tensor \( E^p \), which is supposed
to characterize the current plastic state of the crystal at particle $X$, and that there exists an elastic potential $\phi = \phi(E, E^p)$, such that at any moment during the motion, the stress state at particle $X$ is given by
\[
S = \frac{\partial \phi}{\partial E}(E, E^p) \implies \dot{S} = K : [\dot{E} - K^{-1} K^p : \dot{E}^p] = K : [D - D^{pl}],
\] (3.7)
where the implication follows by taking the time rate of the stress–strain relationship in potential form, and where the following definitions have been used:
\[
K := \frac{\partial^2 \phi}{\partial E \partial E}, \quad K^p := -\frac{\partial^2 \phi}{\partial E \partial E^p} \quad \text{and} \quad D^{pl} := K^{-1} K^p : \dot{E}^p.
\] (3.8)

In general, the equality $D^{pl} = \dot{E}^p$ does not hold, unless $K^p = K$. A sufficient condition for the latter equality to hold is that the elastic potential be of the form $\phi(E, E^p) := \phi^e(E - E^p) + \phi^p(E^p)$. Under the assumption, acceptable at crystal level, that plastic flow does not alter (significantly) the lattice of the crystal and hence its elasticity, throughout the rest of this work, it will be assumed that the elastic potential is independent of the plastic state, that is: $\phi(E, E^p) := \phi^e(E^p)$, where $E^e := E - E^p$. Thus, here, $E^p$ can be regarded as a measure of plastic strain and $E^e$ as a measure of the elastic strain. It is underlined that this intuitive description, in terms of elastic and plastic strains, is not valid in case the structure of the crystal is affected significantly by plastic flow.

Regarding the plastic parameter $E^p$, this will be defined, with respect to the chosen reference configuration $B_0$, as the solution of the Cauchy problem
\[
E^p(X, t) = \dot{D}^{pl} \quad \text{and} \quad E^p(X, t_0) = 0.
\] (3.9)

Once evolution laws have been assigned to the shear rates $\dot{\gamma}^\alpha$, the above problem characterizes uniquely, via equation (3.5), the current value of the plastic parameter $E^p$. This parametrization has the important property that the rate form of the stress–strain relationship in equation (3.7) is a perfect image in the reference configuration of the relationship in equation (2.7) because $D^{pl} = \dot{E}^p = \dot{D}^{pl}$, being thus compatible with the kinematics described in §2. On the other hand, one can imagine many other definitions for $E^p$, each being associated with a corresponding elastic–plastic additive decomposition, and one further example, popular in many investigations based on crystal plasticity, is described in appendix A of this work.

### 4. Slip activation criterion: incorporating non-Schmid effects

The Schmid law states that the slip system $(m^\alpha, n^\alpha)$ is inactive as long as $\tau^\alpha < \tau^\alpha_{ct}$, where $\tau^\alpha := \sigma \cdot (m^\alpha \otimes n^\alpha) = \sigma \cdot n^\alpha$ is the resolved shear stress on the slip system $\alpha$; once $\tau^\alpha$ reaches the critical value $\tau^\alpha_{ct}$, the slip system $\alpha$ becomes (potentially) active. This activation criterion is accurate so long as the motion of the dislocations associated with slip system $\alpha$ is restricted to the slip plane. On the other hand, the motion of dislocations may exhibit deviations from this course. For example, based on atomistic simulations of the motion of $1/2[111]$ screw dislocations, Vitek et al. [14] and Gröger et al. [15] describe a more complex phenomenology of yielding in body-centred cubic lattices, where the non-planar spreading of the dislocation cores leads to violations of the Schmid law; see also the recent review in Bassani & Racherla [21].

More precisely, besides $\tau^\alpha$, other shear components of the stress state are shown to influence the motion of dislocations, and these can lead to the switching of the slip plane (cross-slip). To model these phenomena at crystal level, the cited works employ particular forms of an activation criterion proposed in Qin & Bassani [13], a work, in turn, inspired by the yield behaviour of $L1_2$ intermetallic compounds; Qin & Bassani [13] extend the Schmid law in the form
\[
\sigma \cdot \left( m^\alpha \otimes n^\alpha + \sum_q a^\alpha_q m^\alpha_q \otimes n^\alpha_q \right) \begin{cases} < \tau^\alpha_{ct} & \text{slip system is inactive}, \\ = \tau^\alpha_{ct} & \text{slip system is (potentially) active}, \end{cases}
\] (4.1)
where \( \{m_\alpha^e, n_\alpha^e\} \) are vectors that sample those components of the stress state which may affect the yielding of the crystal and \( a_\alpha^e \)s are scalar constitutive functions. More generally, but retaining the resolved shear stress as the main driving force, the criterion for slip system \( \{n^p, m^p\} \) can be restated as

\[
\sigma \cdot a^e + \zeta^e(\sigma, p) \begin{cases} < \tau_{\text{cr}}^e[1 + \zeta_h^e(\sigma, p_h)], \text{ slip system is inactive,} \\ = \tau_{\text{cr}}^e[1 + \zeta_h^e(\sigma, p_h)], \text{ slip system is (potentially) active,} \end{cases}
\]

(4.2)

where the arguments \( p \) and \( p_h \) incorporate all the additional structural parameters that \( \zeta^e \) and \( \zeta_h^e \) may depend upon, e.g. the \( \{m_\alpha^e, n_\alpha^e\} \) vectors. The functions \( \zeta^e \) represent the contribution of the stress components affecting the configuration of the dislocation cores, whereas \( \zeta_h^e \) represent deviations that may be related to the hardening state of the crystal. For example, for \( \zeta^e \equiv 0 \) and \( \zeta_h^e(\sigma, p_h) = \zeta(\sigma) := -q \text{ tr}(\sigma) \), with \( q > 0 \) a constant material parameter, one recovers an extension of Schmid’s criterion considered in Soare & Barlat [22] and shown to reproduce at macrolevel the criterion of Spitzig & Richmond [12].

By using the pullback of \( a^e \) in equation (3.4), so that \( \tau^e = \sigma \cdot a^e = (1/J)S \cdot A^p \), the extension in equation (4.2) is reformulated in the reference configuration as follows:

\[
S \cdot A^p + \hat{\zeta}^e(S, P) \leq \tau_{\text{cr}}^e[1 + \hat{\zeta}_h^e(S, P_h)],
\]

(4.3)

where \( \hat{\zeta}^e(S, P) := \zeta^e(FSF^T, FpF^T) \), etc. It is assumed that \( \zeta^e \) and \( \zeta_h^e \) are objective functions (like those in equation (4.1)), so that the functions \( \hat{\zeta}^e \) and \( \hat{\zeta}_h^e \) are well defined (invariant to any superimposed rotation).

The above extension will be more convenient for the next derivations because it does not depend explicitly on the volumetric part \( J \). However, strictly speaking, if \( \zeta^e \equiv 0 \) and \( \zeta_h^e \equiv 0 \) are to yield the classical Schmid law, the two activation criteria in equations (4.2) and (4.3) are slightly different. Indeed, in this case, equation (4.3) reads in the current configuration: \( \sigma \cdot a^e \leq \tau_{\text{cr}}^e/J \). Thus, the criterion in equation (4.3) features an additional pressure dependence by comparison with the classical Schmid criteria. Arguments for substituting the Cauchy stress with the Kirchhoff stress in the activation criterion are given in Soare [10]; these show that equation (4.3) is a valid extension of the Schmid law when other non-Schmid effects, represented by the functions \( \zeta^e \) and \( \zeta_h^e \), are neglected.

Finally, considering the thermodynamic consistency of the present model, let us note that, by using equations (3.5) and (4.3), during plastic flow,

\[
S \cdot \mathbf{D}^{PL} = \sum_{\alpha \in A} \gamma^\alpha [J \tau^\alpha + (K^{-1} : S) \cdot (SH^\alpha S + H^\alpha S)].
\]

(4.4)

In general, for the stress levels sustained by metals, the second term between the square brackets is much smaller than the first, see also appendix A for its analysis and it can be concluded that \( S \cdot \mathbf{D}^{PL} > 0 \). Let us note also that in the present framework, the resolved shear stress \( \tau^\alpha \) can be interpreted as a thermodynamic force conjugate to the corresponding shear displacement \( \gamma^\alpha \) only modulo an elastic slip system distortion (the second term between the square brackets). This relaxes the stronger assumption in Rice [7] that \( \tau^\alpha \) be precisely conjugate to \( \gamma^\alpha \).

### 5. Flow rule

Next, the relationship between the direction of plastic flow and the yielding (or activation) surface of the crystal is investigated. Following a convention in Hill & Rice [16], see also Soare [10], the symbol \( \delta \) will be used in this work to denote the \( \theta \)-time rate of an object along an elastic deformation history at its starting point, \( \theta = 0 \), while keeping the reference particle fixed. Thus,

\[
\delta S := \lim_{\theta \to 0} \frac{1}{\theta} [S^\theta - S(0)]
\]

(5.1)
signifies an elastic (stress) direction if \( S^\theta := S(t + \theta), \theta > 0 \), is an elastic stress trajectory for at least some interval \((0, \theta_M) \ni \theta\), with \( \theta_M > 0 \). Then, taking the \( \theta \)-time rate of the elastic stress–strain relationship in equation (3.7), in potential form, gives

\[
\delta S = K : \delta E = \left( \frac{1}{2} \right) K : \delta C. \tag{5.2}
\]

Conversely, for any elastic direction \( \delta S \), there exists an elastic trajectory \( S^\theta \) that has \( \delta S \) as its rate at \( \theta = 0 \).

Let \( S := S(t) \) represent the current stress; assuming that at \( t \) the crystal is in a state of plastic deformation, consider next an arbitrary elastic trajectory \( S^\theta = S(t + \theta), \theta > 0 \), originating at the current stress \( S \). Using equation (4.3),

\[
\frac{S^\theta \cdot (A^\alpha S^\theta + \tilde{\chi}^a(S^\theta, P^\alpha))}{1 + \tilde{\chi}_b^a(S^\theta, P_b^\alpha)} < \tau_{cr}^\alpha = \frac{S \cdot A^\alpha + \tilde{\chi}^a(S, P)}{1 + \tilde{\chi}^b_h(S, P_h^b)},
\]

whence by dividing by \( \theta \) and taking the limit \( \theta \to 0 \),

\[
\delta \left[ \frac{S \cdot A^\alpha + \tilde{\chi}^a(S, P)}{1 + \tilde{\chi}^b_h(S, P_h^b)} \right] \leq 0 \iff \delta[S \cdot A^\alpha + \tilde{\chi}^a(S, P)] - \tau_{cr}^a \delta[\tilde{\chi}^a_h(S, P_h^b)] \leq 0. \tag{5.3}
\]

With \( C = F^T F = F^T C^* F^\alpha, \delta C^a = F^\alpha - T \delta C F^\alpha \) follows, and then, by using equation (5.2),

\[
\delta A^\alpha = \left( \frac{1}{2} \right) (\delta C H^a + H^a T \delta C) = \left( K^{-1} : \delta S \right) H^a + H^a T \left( K^{-1} : \delta S \right), \tag{5.4}
\]

where \( H^a \) was defined in equation (3.6). Because the parameters assembled in \( P \) are, in general, tensor products among vectors associated with the lattice, as in equation (4.1), then, similar to the above formula for \( A^\alpha \), one can assume without loss of generality that there exist tensors \( B \) and \( B_h \) of adequate dimensions such that \( \delta P = B : \delta S \) and \( \delta P_h = B_h : \delta S \). Then, one can write

\[
\delta[\tilde{\chi}^a_h(S, P_h^b)] = \Pi^\alpha_h : \delta S, \quad \text{where} \quad \Pi^\alpha_h := \frac{\partial \tilde{\chi}^a_h}{\partial S} + B^T : \frac{\partial \tilde{\chi}^a_h}{\partial P^\alpha}, \tag{5.5}
\]

and

\[
\delta[\tilde{\chi}^a(S, P)] = \Pi^\alpha : \delta S, \quad \text{where} \quad \Pi^\alpha := \frac{\partial \tilde{\chi}^a}{\partial S} + B^T : \frac{\partial \tilde{\chi}^a}{\partial P^\alpha}. \tag{5.6}
\]

Substituting equations (5.4)–(5.6) into equation (5.3), it may be deduced, by the symmetry of \( K^{-1} \), that for every active slip system,

\[
\delta S \cdot (A^\alpha + K^{-1} : \tilde{H}^a + \Pi^\alpha_h + \tau_{cr}^a \Pi^\alpha_h) \leq 0, \quad \text{with} \quad \tilde{H}^a := S H^a T + H^a S. \tag{5.7}
\]

Multiplying, for each \( \alpha \in \mathcal{A} \), the above inequality with the corresponding shear rate \( \dot{\gamma}^a \) and then summing over the set of active slip systems, we finally deduce, by using equation (3.5),

\[
\delta S \cdot (\dot{D} + Z) \leq 0, \quad \text{where} \quad Z := \sum_{\alpha \in \mathcal{A}} \dot{\gamma}^a (\Pi^\alpha + \tau_{cr}^a \Pi^\alpha_h). \tag{5.7}
\]

The above inequality is valid for arbitrary elastic directions \( \delta S \) issued at the current yielding stress \( S \). As such, it is equivalent to a flow rule: the bracketed object lies within the normal cone to the activation surface of the crystal, at the current stress. One may also note that the elastic variation \( \delta A^\alpha \) depends essentially on the evolution law assigned to the slip systems of the crystal. As such, under the assumptions in equations (3.3) and (3.9), inequality (5.7) is optimal: the only source for deviations from the classical normality rule are the non-Schmid effects. Other forms of slip system evolution, or other parametrizations of the plastic state, lead, in general, to additional deviations from the normal cone to the activation surface ([10]; see appendix A).

### 6. Overall characteristics: elastic potential and flow rule

The next goal is to deduce the essential, in the sense of Hill [23], structure of the overall response of a polycrystal whose constituents feature the just-described constitutive response. This will
be performed here by estimating the response of the polycrystal when subjected to uniform (or homogeneous) displacement boundary conditions. The general framework for averaging material properties is as described in Hill [9]; further details can be found in Nemat-Nasser [24].

Consider an aggregate of single crystals, each constituent being characterized by its orientation with respect to the global Cartesian frame in the reference configuration of the aggregate and by its constitutive response as described earlier. The response of the aggregate is to represent the constitutive response of a macroparticle $\bar{X}$, which is subjected to the macrodeformation gradient $\bar{F}$. With $F(X, t)$ denoting the field of deformation gradient within the aggregate, let $T := r F^T = FS$ denote the corresponding non-symmetric Piola–Kirchhoff (PK), or nominal, stress field. The motion of the aggregate is viewed as a sequence of equilibrium states that are governed by the following equations:

$$\text{div} \ T(X, t) = 0, \quad X \in \Omega, \quad (6.1)$$

$$T(X, t) = F(X, t) \frac{\partial \phi}{\partial E}(X, E, E^p), \quad X \in \Omega, \quad (6.2)$$

and

$$\hat{\chi}(X, t) = \bar{F}(t) \cdot X, \quad X \in \partial \Omega, \quad (6.3)$$

where $X$ is now an explicit argument of the elastic potential because the constituents may be elastically anisotropic, and $\Omega$ is the domain occupied by the aggregate in the reference configuration. Under these conditions, the overall deformation gradient is the direct average of the corresponding field inside the representative volume element, and the overall nominal stress $\bar{T}$ is then defined as the direct average of the local stress field,

$$\bar{F} = \frac{1}{|\Omega|} \int_{\Omega} F(X, t) \, dX \quad \text{and} \quad \bar{T}(t) := \frac{1}{|\Omega|} \int_{\Omega} T(X, t) \, dX, \quad (6.4)$$

where $|\Omega|$ represents the volume of the domain $\Omega$. The local nominal stress field also satisfies the moment of momentum equilibrium in the form $FT = TF$. Averaging this identity over the domain of the aggregate, and taking into account that $T$ is equilibrated and $F$ is compatible (as it is the gradient of $\hat{\chi}$), by Hill’s lemma, it follows that $\bar{F}T = \bar{T} \bar{F}$. Hill’s lemma also applies to the equilibrated and compatible fields $T$ and $\bar{F}$, respectively, and hence

$$\frac{1}{|\Omega|} \int_{\Omega} T \cdot \bar{F} \, dX = \bar{T} \cdot \bar{F}. \quad (6.5)$$

To $\bar{F}$, one can associate an overall Green strain $\bar{E}$ and a corresponding overall symmetric (by the overall moment of momentum equilibrium) PK stress $\bar{S}$, which is defined by requiring that the pairs $(\bar{S}, \bar{E})$ and $(\bar{T}, \bar{F})$ be work conjugated,

$$\bar{E} := \frac{1}{2} (\bar{F}^T \bar{F} - I) \quad \text{and} \quad \bar{S} := \bar{F}^{-1} \bar{T}. \quad (6.6)$$

(a) **Macroelastic potential and macrorate of plastic deformation**

By definition, the aggregate is subjected to elastic deformation if all of its constituents experience elastic deformation. Assume the current stress state is elastic; then, given an arbitrary overall direction of motion $\bar{F}$, there exists a time interval, no matter how small, during which the deformation in this direction remains elastic. Then, with $S$ representing the symmetric PK stress field within the aggregate and $\phi$ the elastic potential, taking into account that the plastic state of the aggregate does not vary during an elastic process, we have, by using equation (6.5),

$$\bar{S} \cdot \bar{E} = \bar{T} \cdot \bar{F} = \frac{1}{|\Omega|} \int_{\Omega} T \cdot \bar{F} \, dX = \frac{1}{|\Omega|} \int_{\Omega} S \cdot \bar{E} \, dX = \frac{d}{dt} \frac{1}{|\Omega|} \int_{\Omega} \phi(X, E, E^p) \, dX. \quad (6.7)$$

Following Hill & Rice [16], we define

$$\tilde{\phi}(\bar{X}, \bar{E}, \bar{H}) := \frac{1}{|\Omega|} \int_{\Omega} \phi(X, E, E^p) \, dX = \frac{1}{|\Omega|} \int_{\Omega} \phi^e(X, E - E^p) \, dX. \quad (6.8)$$
We call the calculations explicit, the general homogenization context will be momentarily relaxed. Contact with the traditional approach to parametrizing the plastic macrostate. However, to make from where it follows, by recalling that $\bar{S} \cdot \tilde{D} = (1/|\Omega|) \int_{\Omega} \bar{S} \cdot D \, dX$,}

\[
\frac{\partial \tilde{\phi}}{\partial \tilde{H}} \cdot \tilde{H} = \frac{-1}{|\Omega|} \int_{\Omega} \bar{S} \cdot \tilde{D}^{PL} \, dX.
\]

Equations (6.10), (6.12) and (6.13) are the basis for the specification of the parameters collected under the abstract notation $\bar{H}$. An illustration will be instructive because it will allow us to make contact with the traditional approach to parametrizing the plastic macrostate. However, to make the calculations explicit, the general homogenization context will be momentarily relaxed.

Illustration. Taylor’s [2] homogenization principle states, based on compatibility reasons, that the deformation is uniform within each constituent and equal to the deformation at the boundary of the aggregate. In the present formalism, this amounts to assuming that $M(\bar{X}, \tilde{E}, \bar{H}) = \bar{E}$, $\forall \bar{X} \in \Omega$, thus disregarding any equilibrium considerations within the aggregate. Then, by equations (6.10)
and (6.9),
\[
\mathcal{S} = \frac{1}{|\Omega|} \int_\Omega \left( \frac{\partial M}{\partial E} \right)^T : \frac{\partial \phi}{\partial E}(X,E,E^p) \, dX.
\]

In addition, for the sake of simplicity, assume that the local elastic potential is the quadratic \( \phi^c(E-E^p) = \frac{1}{2}[K:(E-E^p)] \cdot (E-E^p) \). Then, straightforward calculations, starting from equation (6.8), give
\[
\dot{\phi}(\dot{E},H) = \frac{1}{2}(\ddot{K} \cdot \dot{E} - \dot{K} \cdot \ddot{E}) \cdot \dot{E} + \frac{1}{2} \ddot{E}^p,
\]
where
\[
\ddot{K} := \frac{1}{|\Omega|} \int_\Omega K \, dX, \quad \ddot{E}^p := \frac{1}{|\Omega|} \int_\Omega \ddot{K}^{-1} K : E^p \, dX
\]
and
\[
\ddot{E}^p := \frac{1}{|\Omega|} \int_\Omega (K : E^p) \cdot E^p \, dX.
\]

We show that \( H := (\ddot{E}^p, \ddot{E}^p) \) is a valid parametrization of the plastic state of the aggregate. First, let us note that \( \ddot{E}^p \) and \( \ddot{E}^p \) are independent entities (for example, \( \ddot{E}^p \) may be constant in situations where \( \ddot{E}^p \) varies). Then, using equations (6.14)–(6.15),
\[
\mathcal{S} = \frac{1}{|\Omega|} \int_\Omega \left( \frac{\partial \phi^c}{\partial E} \right) \, dX = \frac{1}{|\Omega|} \int_\Omega K : (\dot{E} - \dot{E}^p) \, dX = \ddot{K}^{-1} K : E^p \, dX
\]
and hence equation (6.10) is verified. Next, by equation (6.12) and equation (6.28) below, the following must hold:
\[
\ddot{E}^p : \dot{H} = \ddot{D}^p = \frac{1}{|\Omega|} \int_\Omega \ddot{K}^{-1} K : E^p \, dX \quad \Leftrightarrow \quad \ddot{E}^p : \dot{H} = \ddot{E}.
\]

Recalling the definitions in equation (6.12), one has \( \ddot{E}^p = [\ddot{K}, 0] \) and \( \dot{H} = [\ddot{E}^p, \ddot{E}^p] \); hence, the above identity is also satisfied. Finally,
\[
\frac{\partial \ddot{E}^p}{\partial \ddot{E}^p} \cdot \dot{\ddot{E}}^p + \frac{\partial \ddot{E}^p}{\partial \ddot{E}^p} \cdot \ddot{E}^p = -(\ddot{K} \cdot \dot{E} - \dot{K} \cdot \ddot{E}) + \frac{1}{|\Omega|} \int_\Omega (K : E^p) \cdot E^p \, dX = -\frac{1}{|\Omega|} \int_\Omega S : \ddot{D}^p \, dX,
\]
and hence the identity in equation (6.13) is verified, thus closing our proof.

Some of the features of the above example extend to the general case. Indeed, having defined a macrorate of plastic deformation, by equations (6.11) and (6.12), one can always associate with it a measure of plastic deformation in the form of the symmetric second-order tensor \( \mathcal{E}(X,t) \) solution of the Cauchy problem
\[
\dot{E}^p = \ddot{D}^p, \quad \text{with } \mathcal{E}(X,t_0) = 0.
\]

Then, a parametrization of the plastic state may be given in the form \( H = (\ddot{E}^p, Q) \), where \( Q \) denotes a set of any additional plastic parameters. With \( \bar{\phi} = \phi(E, \ddot{E}^p, Q) \), equation (6.13) can be rewritten as
\[
\frac{\partial \bar{\phi}}{\partial E^p} \cdot \dot{E}^p + \frac{\partial \bar{\phi}}{\partial Q} \cdot Q = \frac{1}{|\Omega|} \int_\Omega \ddot{D}^p \cdot S \, dX.
\]

Formally, nothing seems to prevent the consideration of a macrostress potential of the form \( \bar{\phi}(E, \ddot{E}^p, Q) = \phi(E, Q) \), with \( \ddot{E}^p := \ddot{E} - \ddot{E}^p \) and possibly different characterizations of the \( Q \)-parameters of the \( \bar{\phi} \) function. However, in this case, the presence of the additional parameters \( Q \) is mandatory. Indeed, if these were absent, then owing to the relationship \( \partial \bar{\phi}/\partial E^p = -\partial \bar{\phi}/\partial E^e = -\mathcal{S} \), the above identity would reduce to
\[
\mathcal{S} : \ddot{D}^p = \frac{1}{|\Omega|} \int_\Omega \ddot{D}^p \cdot S \, dX.
\]

This dissipation identity is false, in general; by equation (6.28), an identity of this type holds, in general, only for elastic directions.
(b) Macroyield surface

The elastic domain at the continuum particle $X$ is defined as the set of all macrostresses $S^e$ that can be reached from the current stress $\bar{S}$ by elastic deformation of the aggregate [23]. The overall stress associated with an elastic process starting at $\bar{F}$, the deformation gradient at the current moment $t$, and ending at $\bar{F}^e$ is

$$\bar{S}^e = \frac{\partial \phi}{\partial \bar{E}}(\bar{E}^e, H),$$

(6.17)

with $\bar{E}^e$ denoting the Green strain associated with $\bar{F}^e$. It is assumed that the single-crystal potential is strictly convex and co-finite [26], so that by equation (6.8), the overall potential $\phi$ is also strictly convex and co-finite. Under these conditions, the above stress–strain relationship can be inverted in the form

$$\bar{E}^e = \frac{\partial \psi}{\partial \bar{S}}(\bar{S}^e, H),$$

with $\psi(\bar{S}, H) := \bar{S} \cdot \bar{E} - \phi(\bar{E}, H)$.

(6.18)

The local stress field $S^e$ can now be calculated in terms of the overall stress $\bar{S}^e$ via equations (3.7) and (6.9). Then, equation (4.3) leads to the following set of inequalities to be satisfied by $\bar{S}^e$:

$$\frac{\partial \phi}{\partial \bar{E}}(M(X, \bar{E}^e, H), E^p) \cdot A^a + \hat{\zeta}^a \left( \frac{\partial \phi}{\partial \bar{E}}(M(X, \bar{E}^e, H), E^p), P \right) < \tau_{\text{ct}} \left[ 1 + \hat{\zeta}^a \left( \frac{\partial \phi}{\partial \bar{E}}(M(X, \bar{E}^e, H), E^p), P \right) \right],$$

(6.19)

for all $a \in S$ and every $X \in \Omega$, where $\bar{E}^e$ is given by equation (6.18) and $A^a$ also depend on the current stress state via equation (3.4). In general, it cannot be expected that the set defined by each of the above inequalities be convex, see appendix A for a counterexample. On the other hand, deviations from convexity are so small that one may assume, without much loss in rigour, that the intersection of the sets defined by the above set of inequalities is convex.

Based on the above inequalities, it will be assumed that the macroelastic domain can be characterized by using a yield function $f$ in the form

$$f(\bar{S}^e, \ldots) = g_\tau(\bar{S}^e, \ldots) + g_t(\bar{S}^e, \ldots) - h(\ldots)g_r(\bar{S}^e, \ldots) < 0,$$

(6.20)

where $\tau(\bar{S}^e, \ldots) := g_\tau(\bar{S}^e, \ldots) + g_t(\bar{S}^e, \ldots)$ is representative of the left-hand side of the inequality in equation (6.19), and referred to as the equivalent macrostress; $g_\tau(\bar{S}^e, \ldots)$ is representative of the left-hand side if the contributions of $\hat{\zeta}^a$ in equation (6.19) were absent; $h(\ldots)g_r(\bar{S}^e, \ldots)$ is to represent the right-hand side, and is referred to as the hardening part of the macroyield function. Only the macrostress has been shown explicitly as the argument because this will be relevant for our next developments; the dots are to represent any additional (structural) parameters that may be required for characterizing the shape and symmetries of the macroelastic domain, or its size. The macroyield surface is, by definition, the boundary of the macroelastic domain; it is characterized by $f(\bar{S}^e, \ldots) = 0$.

(c) Macroflow rule

Consider an arbitrary elastic direction of motion, originating at the current moment $t$; this is a velocity field $\delta \hat{x}$ for which there exists a time interval such that continuing the motion in this direction would induce an elastic state within the aggregate [10]. It is characterized by the following BVPs, obtained by linearizing BVPs (6.1)–(6.3) at $t$ with a fixed plastic state:

$$\text{div} \delta T(X) = 0, \quad X \in \Omega,$$

$$\delta T(X) = [\delta F(X)] S(X, t) + F(X, t) K : \delta E(X), \quad X \in \Omega,$$

and

$$\delta \hat{x}(X) = \delta \hat{F} : X, \quad X \in \partial \Omega.$$

(6.21)

Corresponding macroelastic directions are defined as

$$\delta \bar{E} := \frac{1}{2} \left( (\delta \hat{F})^T \hat{F}(t) + \hat{F}(t) (\delta \hat{F}) \right) \text{ and } \delta \bar{S} := \bar{K} : \delta \bar{E},$$

(6.22)
with \( \bar{K} \) defined in equation (6.12). During the virtual (or \( \theta \))-motion relationship (6.9) continues to hold and hence, by taking the \( \theta \)-time rate, at \( \theta = 0 \), the local strain and stress fields are determined by the macrostrain and stress increments as follows:

\[
\delta E(X) = G_M : \delta \bar{E} \implies \delta S = K : \delta E = KG_M : \delta \bar{E} = KGM\bar{K}^{(-1)} : \delta \bar{S},
\]

(6.23)

where

\[
G_M(X, \bar{E}, H) := \frac{\partial M}{\partial \bar{E}} (X, \bar{E}, H).
\]

(6.24)

Next, by using the local stress–strain relationship in equation (3.7) and the symmetry of \( K \),

\[
\delta S \cdot D^{pl} = \delta S \cdot (D - K^{-1} : \delta \bar{S}) = \delta S \cdot D - (K^{-1} : \delta S) \cdot \bar{S} = \delta S \cdot D - \delta E \cdot \bar{S}.
\]

(6.25)

The last member in the above sequence of equalities is an instance of Hill’s differential form [9,27]. This form has the remarkable property that it is invariant to changes of conjugate stress–

strain measures. For our purpose, the conjugate pair \((T, F)\) is of primary interest; it is related to the pair \((S, E)\) by: \( T = FS \implies \delta T = (\delta F)S + F\delta S \), and \( T = FS + FS; \ E = (\frac{1}{2})(F^TF - I) \implies \delta E = (\frac{1}{2})(\delta F^TF + F^T\delta F) \). With these relationships, the following identity is easily verified:

\[
\delta S \cdot D - \delta \bar{S} \cdot \delta E = \delta T \cdot \bar{F} - \bar{T} \cdot \delta F.
\]

(6.26)

Now, \( (\delta T, \bar{F}) \) and \( (\bar{T}, \delta F) \) are pairs of equilibrated and compatible fields, and hence an average relationship such as equation (6.5) holds for each. Then, averaging in (6.25) and using (6.26), gives

\[
\frac{1}{|\Omega|} \int_{\Omega} \delta S \cdot D^{pl} \, dX = (\delta \bar{T}) \cdot \bar{F} - \bar{T} \cdot \delta \bar{F} = (\delta \bar{S}) \cdot \bar{D} - \bar{S} \cdot \delta \bar{E}
\]

\[
= \delta \bar{S} \cdot (\bar{D} - \bar{K}^{(-1)} : \bar{S}).
\]

(6.27)

Using equation (6.11), the bracketed term on the right of the last equality above is the macrorate of plastic deformation, \( \dot{D}^{pl} \). Then, by substituting in the integral term above, the relationship in equation (6.23) between the local and macroelastic stress directions, one obtains an identity valid for arbitrary \( \delta \bar{S} \), leading to the following representation of the macrorate of plastic deformation:

\[
\dot{D}^{pl} = \frac{1}{|\Omega|} \int_{\Omega} \bar{K}^{(-1)}(G_M)^T K : D^{pl} \, dX.
\]

(6.28)

Averaging over the domain of the aggregate the inequality in equation (5.7), and using equations (6.28) and (6.23), results in the inequality

\[
\bar{S} \cdot (\bar{D}^{pl} + \bar{Z}) \leq 0, \quad \text{with } \bar{Z} := \frac{1}{|\Omega|} \int_{\Omega} \bar{K}^{(-1)}(G_M)^T K : Z \, dX,
\]

(6.29)

valid for any macroelastic direction \( \delta \bar{S} \). Assuming the macroyield function is smooth, the above inequality then translates into the following flow rule:

\[
\bar{D}^{pl} + \bar{Z} = \dot{\lambda} \frac{\partial f}{\partial \bar{S}}(\bar{S}, \ldots),
\]

(6.30)

with \( \dot{\lambda} \) denoting a scalar parameter characterizing the magnitude of \( \bar{D}^{pl} + \bar{Z} \).

(d) Eulerian description

Since many of the current investigations in metal plasticity use a hypoelastic formulation of the stress–strain response, it is perhaps not without relevance to rephrase the essence of the above results in terms of spatial objects (defined on the current configuration of the continuum body).

With \( S \) and \( \tau := |\sigma| \) (re)denoting the symmetric PK and, respectively, the Kirchhoff macrostresses, the stress–strain relationship, in the rate form of equation (6.11), reads, in the
reference and current configurations,
\[
\dot{S} = K : [D - D^{pl}] \iff \dot{\iota}^1 = K^1 : [d - d^{pl}] \iff \dot{\iota}^1 = K^1 : [d - d^p],
\]
where \( d \) is the Eulerian macrorate of deformation, i.e. the symmetric part of the spatial velocity gradient \( I, F \) the macrodeformation gradient, \( D = F^T d F, D^{pl} = F^T d^{pl} F, K^1 : a = F[K : (F^T a F)]F^T \), for any symmetric \( a, \dot{\iota}^1 = \dot{\iota} - l r - \tau^I, \dot{\iota}^1 = \dot{\iota} + \tau w - w r, w := (I - I^T)/2, K^1 : a = K^1 : a + \tau a + a \tau, \) for any symmetric \( a, \) and \( d^p := (K^0)^{-1} K^1 : d^{pl} \).

In the context of §6b, let \( \Delta F^e = F F^{-1} \) denote the macrodeformation gradient of an arbitrary macroelastic deformation starting from the current configuration defined by the macrodeformation gradient \( F \). With the polar decomposition \( \Delta F^e = RU \), for any elastic stress state \( S^e, S^0 = F^{-1} \tau F^{-T} = F^{-1} l U^{-1} \tau F^{-T}, \) holds, where \( \tau^R := R^T \tau R. \) Because the deformation is elastic, \( S^e \) and \( U \) are in a one-to-one relationship and hence \( \tau^R \) and \( S^0 \) are also in a one-to-one relationship. One can then define \( f^e(\tau^R, \ldots) := f^S(F^{-1} l U^{-1} \tau F^{-T}, \ldots), \) with \( f^S \) now denoting the overall yield surface defined in equation (6.20). Letting \( Q \) denote the rotation associated with the material spin, \( \dot{Q} = \omega Q, \) a further definition of the macroyield function written with respect to axes that spin with \( \omega, f^Q(\tau^Q, \ldots) := f^e(\tau^R, \ldots), \) allows us to characterize the elastic domain in the form \( f^Q(\tau^Q, \ldots) < 0; \) also, by defining \( f(\tau, \ldots) := f^Q(\tau^Q, \ldots), \) one can reformulate this characterization in terms of the Kirchhoff stress itself by writing \( f(\tau, \ldots) < 0. \) In the latter case, it is implied that, for anisotropic yielding properties, the arguments of \( f \) include some characteristic structural tensors \([28,29] \), for otherwise the principle of objectivity would restrict \( f \) to an isotropic function.

With \( f^Q(\tau^Q, \ldots) \) describing the elastic domain, its elastic directions, issued at the current stress \( \tau, \) are of the form \( \delta \tau^Q = Q^T (\delta \tau + \tau w - w r) Q = Q^T (\delta^l \tau) Q, \) the latter equality serving as a definition of the operator \( \delta^l. \) Along elastic directions, \( \delta^l \tau = K^1 : d \) holds, and then \( \delta^l \) is related to \( \delta^l \tau := \delta \tau - l r - \tau^I \) by \( \delta^l \tau = N : \delta^l \tau, \) with \( N : a = a + \tau (K^1)^{-1} : a + [(K^1)^{-1} : a] \tau, \) for any symmetric second-order tensor \( a. \) The N-operator relates also the two spatial plastic rates in equation (6.31) by \( d^{pl} = N^T : d^p. \) Then, with equation (6.29),
\[
0 \geq \delta S \cdot (D^{pl} + \tilde{Z}) = \delta \tau^L \cdot (d^{pl} + z^L) = \delta^l \tau \cdot (d^p + z) = \delta \tau^Q \cdot [Q^T (d^p + z) Q],
\]
where \( z^L := F^{-T} \tilde{Z} F^{-1} \) and \( z := N^{-T} : z^L. \) With \( \delta \tau^Q \) arbitrary, from the last inequality above,
\[
d^p + z = \dot{k} Q \frac{\partial f^Q}{\partial \tau} Q^T = \dot{\lambda} \frac{\partial f}{\partial \tau}.
\]
This is the Eulerian form of the flow rule in equation (6.30). When non-Schmid effects are absent, it reduces to the classical normality rule.

Finally, let us note that by the definition of \( \tilde{Z} \) and \( Z \) in equations (6.29) and (5.7), the deviation from the normal direction can be decomposed as \( z = z_1 + z_r, \) where \( z_1 \) is representative of \( \zeta^0 \) (or ‘left-hand’) effects, whereas \( z_r \) is representative of \( \zeta^0 \) (or ‘right-hand’) effects; also, by equation (6.20), the yield function admits the Eulerian representation \( f(\tau, \ldots) = g_r(\tau, \ldots) + g_l(\tau, \ldots) - h(\ldots) g_l(\tau, \ldots). \) Then, the flow rule in equation (6.32) can be further specified in the form
\[
d^p + z_1 + z_r = \dot{k} \left( \frac{\partial g_r}{\partial \tau} + \frac{\partial g_l}{\partial \tau} - h \frac{\partial g_r}{\partial \tau} \right).
\]

7. Conclusion

The overall response of a polycrystal, representative of a continuum particle \( X, \) has been analysed here under the following conditions: (i) the stress–strain response of a constituent crystal derives from an elastic potential; (ii) the slip systems of a constituent convect with the crystal lattice; and (iii) an extended Schmid law, incorporating non-Schmid effects, characterizes slip activity. Then, a macroelastic potential \( \Phi = \Phi(E, H) \) exists, Hill & Rice [16], such that the response at particle \( X \) is
where $S$ and $E$ are the symmetric PK stress and the Green strain with respect to a reference configuration. $H$ is a collection of variables that parametrize the current plastic state at particle $X$. A macroyield function exists and describes the elastic domain at particle $X$. A macroyield function exists and describes the plastic state of a single crystal, based on the supposedly more intuitive and hence a priori concept of elastic (or plastic) strain. Its details and consequences at macrolevel are examined next.

(a) An additive elastic–plastic decomposition

The context being that of equation (3.1), the Green strain

$$E^* := \frac{1}{2}(C^* - I), \quad \text{with } C^* := F^{*T}F^*,$$

is adopted as a measure of the elastic strain between the intermediate and current configurations. To define its image (or pullback) $E^e$ in the reference configuration, let $dX \in TX$ be an arbitrary vector with its image $dx = F : dX = F^e : dXP$; with $dl_p$ and $dl$ denoting the lengths of $dX$ in the intermediate and current configurations,

$$(E^e : dX) \cdot dX := \frac{(dl^2 - dl_p^2)}{2} = (E^* : dXP) \cdot dXP.$$  \hspace{1cm} (A 2)

With $dXP = FP : dX,$

$$E^e = FP^T E^* F^p = \frac{1}{2}(C - C^p) = E - E^p, \quad C := F^T F \quad \text{and} \quad C^p := F^{pT}F^p,$$

and the total and plastic Green strain tensors $E$ and $E^p$ are defined by

$$E := \frac{1}{2}(C - I) \quad \text{and} \quad E^p := \frac{1}{2}(C^p - I).$$

The additive decomposition in equation (A 3), i.e. $E = E^e + E^p$, was postulated in the pioneering work of Green & Naghdi [30] on macroplasticity theory at finite strain. Using the above arguments, it is equivalent with the multiplicative decomposition in equation (3.1). However, one may note that this decomposition differs from the one associated with the plastic parameter defined in equation (3.9). One may also note that both $E^p$ and $E^e$ are invariant to any orthogonal transformation of the intermediate configuration, hence, the advantage of using a Lagrangian formulation based on the reference state over a Lagrangian formulation based on the intermediate...
configuration, the latter being prominent in many of the recent works on crystal plasticity; see also the discussion in Green & Naghdi [31].

Equation (A 5) reproduces the basic features of small strain elasticity, appropriate for metals, when \( \tilde{e} \) is in a small vicinity of \( 0 \). It is remarked that in the cited works, \( E^e \), as defined by equation (A 1), is used as the primary elastic strain measure, and the symmetric PK stress \( S^e := F^{e-1} \sigma F^{e-T} \) as the stress measure in the intermediate configuration, to define the elastic law in the form \( S^e = K : E^e \). This relationship can be obtained by the pushforward of equation (A 5) to the intermediate configuration, while assuming, formally, that \( K \) is left unchanged by plastic flow, that is, by \( F^p \).

Then, the rate of plastic deformation takes the form

\[
D^{pl} := \dot{E}^p = F^p \frac{1}{2}(L^P + L^{PT})F^p. \tag{A 6}
\]

Of further interest is its relationship with the rate \( \dot{D}^{pl} \) defined in equation (3.5). To deduce it, one may first note that

\[
D^e := \dot{E}^e = D^\varepsilon + D^\zeta, \quad \text{where} \quad D^\varepsilon := F^{pT}L^PTF^{p-T}E^e + E^e F^{p-1}L^PF^p, \tag{A 7}
\]

and where \( D^\varepsilon := F^T d^a F \), with the Euler rates \( d^a = d^a \) defined in equations (3.2) and (2.1). Then, \( D^{pl} = D - D^e = D - (D^\varepsilon + D^\zeta) = D - (D - D^p + D^\varepsilon) = D^p - D^\varepsilon \); recalling the relationship in equation (3.5) and, for the sake of simplicity, using the stress–strain relationship in equation (A 5) gives

\[
D^{pl} = \dot{D}^{pl} - D^{2pl},
\]

where

\[
D^{2pl} := K^{-1} : (\dot{L}^P S + S\dot{L}^{PT}) + (K^{-1} : S)\dot{L}^P + \dot{L}^{PT}(K^{-1} : S)
\]

and where, for more compact writing, the definition \( \dot{L}^P := F^{p-1}L^PF^p \) has been used.

(b) A study of the convexity of the activation surface

With slip systems evolving according to equation (3.3), the activation surface of the crystal is defined by equation (4.3). Because slip directions are embedded into the lattice, they are subjected to the influence of any deformation history and in particular to that of elastic unloading. A consequence of this is that the elastic domain (at a particle of the crystal) is not convex in general.

To show this, it is will be assumed that the stress–strain relationship is given by that in equation (A 5) and that non-Schmid effects are absent. With \( S \) denoting the current stress state, the current elastic domain of the crystal is defined as the set of all stress states \( S^e \) that can be reached starting from \( S \) by a purely elastic deformation process. Let \( F \) and \( F^e \) denote the deformation gradients corresponding to \( S \) and \( S^e \), respectively. With \( S^e \) corresponding to an elastic state, the plastic state of the crystal at \( S \) and \( S^e \) is the same. Then, \( S = K : (C - C^p) / 2 \) and

\[
S^e = \frac{1}{2}K : (C^e - C^p) = S + \frac{1}{2}K : (C^e - C). \tag{A 9}
\]

In addition, it follows that \( F^e = (F^e)^*F^p \) and hence \( C^e := (F^e)^TF^e = F^pT(C^e)^*F^p \). Then, by equation (3.4), the \( A \)-tensor of slip system \( \alpha \) corresponding to the stress state \( S^e \) is given by the
particular, with 6
Then, with
the elastic domain of the crystal is that resulting from the linear part of the activation criterion,
To simplify, let us assume isotropic elastic properties:
φα
The above
valid for any macroelastic direction
where the quadratic term in each inequality reads
φα(S′) + \frac{1}{2} S′ \cdot [(C − 2K^{-1} : S)Hα + HαT(C − 2K^{-1} : S)] < τ_{cr,\alpha},
where the quadratic term in each inequality reads
φα(S′) := (K^{-1} : S′) \cdot (S′HαT + HαS′).
To simplify, let us assume isotropic elastic properties: K^{-1} = αI ⊗ I + bI, with a := −λ/[2μ(3λ + 2μ)] and b := 1/(2μ), in terms of Lame’s parameters. Then,
φα(S′) = [a \text{tr}(S′)S′ + b(S′)^2] \cdot (Hα + HαT).
The above φα is not a convex function. First, let us note some properties of the Hα tensor,
Hα = (FP^{-1} : m^α) ⊗ (FP^T : n^α), \quad \text{tr}(Hα) = 0 \quad \text{and} \quad (Hα + HαT)^2 \cdot Hα = 0.
Then, with S_H := Hα + HαT, one can further calculate
φα(I) = 0, \quad φα(S_H) = 0 \quad \text{and} \quad φα(t_1I + t_2S_H) = (6a + 4b)t_1t_2m^2n^2,
for any reals t_1 and t_2, where the notations m := |FP^{-1} : m^α|, n := |FP^T : n^α| have been used. In particular, with 6α + 4b > 0, when t_1t_2 < 0, it follows that φα(t_1I + t_2S_H) < 0, thus showing that φα is not a positive definite quadratic. More precisely, for each α, the nature of the above quadratic is hyperbolic, and hence the elastic domain of the crystal, as defined by equation (A 11) is not a convex set.

For moderate stresses, the quadratic terms gathered in φα are barely ‘visible’, their amplitudes being several orders smaller than those of the linear terms. In other words, the overall shape of the elastic domain of the crystal is that resulting from the linear part of the activation criterion, while the quadratic terms just superimpose small variations upon it.

(c) Flow rules and pseudo-deviations from normality

In general, the difference between the two rates in equation (A 8) is just a small fraction of the rate of plastic deformation. However, if non-Schmid effects are to be accounted for, then D^{pl} can be neglected only after a comparison with the magnitude of these effects. When D^{pl} cannot be neglected, it is at the origin of an additional source of deviation from the cone of normal directions. Indeed, using equations (5.7) and (A 8) gives
δS \cdot (D^{pl} + D^{pl} + Z) \leq 0,
an inequality valid for any elastic direction δS.
Then, considering an aggregate of single crystals, averaging the above inequality and using equations (6.28) and (6.23), results in the inequality
δ\bar{S} \cdot (\bar{D}^{pl} + \bar{D}^{pl} + \bar{Z}) \leq 0, \quad \text{with} \quad \bar{D}^{pl} := \frac{1}{|Ω|} \int_Ω \bar{K}(-1)(G_M)^T K : D^{pl} \, dX,
valid for any macroelastic direction δ\bar{S}. Assuming the macroyield surface is smooth (and convex), the above inequality then translates into the flow rule
\bar{D}^{pl} + \bar{D}^{pl} + \bar{Z} = \dot{\lambda} \frac{∂f}{∂\bar{S}}(\bar{S}, \ldots),
(A 19)
with $\dot{\lambda}$ denoting a scalar parameter characterizing the magnitude of $\dot{D}^{pl} + \dot{D}^{pL} + \dot{Z}$. With $\dot{D}^{pl}$ representing the macrorate of plastic deformation and $\dot{Z}$ the rate of (intrinsic) non-Schmid effects, the additional term $\dot{D}^{pL}$ represents a pseudo-deviation from normality, induced solely by the chosen parametrization of the plastic state at the constituent level.

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