



# On the partitioning of the rate of deformation gradient in phenomenological plasticity

V.A. Lubarda<sup>\*</sup>, D.J. Benson

*Department of Mechanical and Aerospace Engineering, University of California at San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0411, USA*

Received 28 July 2000; in revised form 28 November 2000

---

## Abstract

The rate of deformation gradient is partitioned additively into its elastic and plastic parts within the framework of phenomenological plasticity based on the multiplicative decomposition of deformation gradient. The corresponding partition of the nonsymmetric nominal stress is also given. The results are compared with the well-known results of partitioning the rates of Lagrangian strain and its conjugate symmetric Piola–Kirchhoff stress. Extension to the framework of monocrystalline plasticity is then discussed. © 2001 Elsevier Science Ltd. All rights reserved.

*Keywords:* Plasticity; Multiplicative decomposition; Rate of deformation gradient; Nominal stress; Elastoplastic partitioning

---

## 1. Introduction

The purpose of this paper is to elaborate on the partition of the rate of deformation gradient and the rate of nonsymmetric nominal stress into their elastic and plastic parts within the framework of phenomenological plasticity based on the multiplicative decomposition of deformation gradient. Such partitions have been previously considered by Hill (1984) and Havner (1992) in the context of micro-to-macro transition and crystalline plasticity, and were found to be particularly useful in the theoretical analysis of inelastic material response.

Consider an elastoplastically deformed configuration of the material sample  $\mathcal{B}$ , whose initial undeformed configuration was  $\mathcal{B}^0$ . Let  $\mathbf{F}$  be the deformation gradient that maps an infinitesimal material element  $d\mathbf{X}$  from  $\mathcal{B}^0$  to  $d\mathbf{x}$  in  $\mathcal{B}$ , such that  $d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X}$ . Introduce the intermediate configuration  $\mathcal{B}^p$  by elastic destressing to zero stress of the configuration  $\mathcal{B}$ . The intermediate configuration differs from the initial configuration by residual (plastic) deformation, and from the elastoplastically deformed configuration by reversible (elastic) deformation. If  $d\mathbf{x}^p$  is the material element in  $\mathcal{B}^p$  corresponding to  $d\mathbf{x}$  in  $\mathcal{B}$ , then  $d\mathbf{x} = \mathbf{F}^e \cdot d\mathbf{x}^p$ , where  $\mathbf{F}^e$  represents the deformation gradient associated with elastic loading from  $\mathcal{B}^p$  to  $\mathcal{B}$ . If

---

<sup>\*</sup> Corresponding author. Tel.: +1-858-534-3169; fax: +1-858-534-5698.

E-mail address: vlubarda@ucsd.edu (V.A. Lubarda).

$\mathbf{F}^p$  is the deformation gradient of the transformation  $\mathcal{B}^0 \rightarrow \mathcal{B}^p$ , such that  $d\mathbf{x}^p = \mathbf{F}^p \cdot d\mathbf{X}$ , the multiplicative decomposition of the total deformation gradient into its elastic and plastic parts follows (Lee, 1969)

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p. \quad (1)$$

For inhomogeneous deformations only  $\mathbf{F}$  is a true deformation gradient, whose components are the partial derivatives  $\partial \mathbf{x} / \partial \mathbf{X}$ . The mappings  $\mathcal{B}^p \rightarrow \mathcal{B}$  and  $\mathcal{B}^0 \rightarrow \mathcal{B}^p$  are not, in general, continuous one-to-one mappings, so that  $\mathbf{F}^e$  and  $\mathbf{F}^p$  are not defined as the gradients of the respective mappings (which may not exist), but as the point functions (local deformation gradients). In the case when elastic destressing to zero stress is not physically achievable due to possible onset of reverse plastic deformation before the state of zero stress is reached, the intermediate configuration can be conceptually introduced by virtual destressing to zero stress, locking all inelastic structural changes that would take place during the actual destressing.

The deformation gradients  $\mathbf{F}^e$  and  $\mathbf{F}^p$  are not uniquely defined, because the intermediate configuration is not unique. Arbitrary local material rotation  $\hat{\mathbf{Q}}$  can be superposed to the intermediate configuration, preserving it unstressed. Thus, we can write

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p = \hat{\mathbf{F}}^e \cdot \hat{\mathbf{F}}^p, \quad (2)$$

where

$$\hat{\mathbf{F}}^e = \mathbf{F}^e \cdot \hat{\mathbf{Q}}^T, \quad \hat{\mathbf{F}}^p = \hat{\mathbf{Q}} \cdot \mathbf{F}^p. \quad (3)$$

In applications the decomposition (1) can be made unique by additional requirements dictated by the nature of the considered material model. For example, for elastically isotropic materials the stress response from  $\mathcal{B}^p$  to  $\mathcal{B}$  depends only on the elastic stretch  $\mathbf{V}^e$ , and not on the rotation  $\mathbf{R}^e$  from the decomposition  $\mathbf{F}^e = \mathbf{V}^e \cdot \mathbf{R}^e$ . Consequently, the intermediate configuration can be specified uniquely by requiring that elastic unloading takes place without rotation,  $\mathbf{F}^e = \mathbf{V}^e$  (Lee, 1969; Lubarda and Lee, 1981). On the other hand, in single crystal plasticity, the orientation of the intermediate configuration is specified by fixed orientation of the crystalline lattice, through which the material flows by crystallographic slip during the transformation from  $\mathcal{B}^0$  to  $\mathcal{B}^p$ . In Mandel's (1973) model, if the triad of orthogonal (director) vectors is attached to initial configuration, and if this triad remains unaltered by plastic deformation, the intermediate configuration is referred to as isoclinic. Such configuration is unique at any given stage of elastoplastic deformation, because a superposed rotation  $\hat{\mathbf{Q}} \neq \mathbf{I}$  would change orientation of the director vectors, and the configuration would not remain isoclinic. Further discussion of nonuniqueness of the decomposition can be found in the articles by Naghdi (1990) and Lubarda (1991). For computational aspects of finite deformation elastoplasticity based on the multiplicative decomposition, see the recent book by Simo and Hughes (1998).

If Lagrangian strains corresponding to deformation gradients  $\mathbf{F}^e$  and  $\mathbf{F}^p$  are defined by

$$\mathbf{E}^e = \frac{1}{2}(\mathbf{C}^e - \mathbf{I}), \quad \mathbf{E}^p = \frac{1}{2}(\mathbf{C}^p - \mathbf{I}), \quad (4)$$

where  $\mathbf{C}^e = \mathbf{F}^{eT} \cdot \mathbf{F}^e$  and  $\mathbf{C}^p = \mathbf{F}^{pT} \cdot \mathbf{F}^p$ , the total Lagrangian strain can be expressed as

$$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I}) = \mathbf{E}^p + \mathbf{F}^{pT} \cdot \mathbf{E}^e \cdot \mathbf{F}^p. \quad (5)$$

The elastic and plastic strains  $\mathbf{E}^e$  and  $\mathbf{E}^p$  do not sum to give the total strain  $\mathbf{E}$ , because  $\mathbf{E}$  and  $\mathbf{E}^p$  are defined relative to the initial configuration  $\mathcal{B}^0$  as the reference, while  $\mathbf{E}^e$  is defined relative to the intermediate configuration  $\mathcal{B}^p$  as the reference. Consequently, it is the strain  $\mathbf{F}^{pT} \cdot \mathbf{E}^e \cdot \mathbf{F}^p$ , induced from the elastic strain  $\mathbf{E}^e$  by plastic deformation  $\mathbf{F}^p$ , that sums up with the plastic strain  $\mathbf{E}^p$  to give the total strain  $\mathbf{E}$ .

The following expressions hold for the rates of Lagrangian strains  $\mathbf{E}^e$  and  $\mathbf{E}^p$ :

$$\dot{\mathbf{E}}^e = \mathbf{F}^{p-T} \cdot \dot{\mathbf{E}} \cdot \mathbf{F}^{p-1} - [\mathbf{C}^e \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1})]_s, \quad (6)$$

$$\dot{\mathbf{E}}^p = \mathbf{F}^{pT} \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1})_s \cdot \mathbf{F}^p. \quad (7)$$

These are conveniently expressed in terms of the strain rate  $\dot{\mathbf{E}}$  and the velocity gradient  $\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1}$ . In general,  $\dot{\mathbf{E}}^e + \dot{\mathbf{E}}^p \neq \dot{\mathbf{E}}$ .

## 2. Partitioning of the rate of Lagrangian strain

It is assumed that the material is elastically isotropic in its initial undeformed state, and that plastic deformation does not affect its elastic properties. The elastic strain energy per unit unstressed volume  $\Psi^e$  is then an isotropic function of the Lagrangian strain  $\mathbf{E}^e$ , which can be expressed as (Lubarda, 1994)

$$\Psi^e = \Psi^e(\mathbf{E}^e) = \Psi^e[\mathbf{F}^{p-T} \cdot (\mathbf{E} - \mathbf{E}^p) \cdot \mathbf{F}^{p-1}]. \quad (8)$$

From this we derive the symmetric Piola–Kirchhoff stress tensors,

$$\mathbf{T}^e = \frac{\partial \Psi^e}{\partial \mathbf{E}^e}, \quad \mathbf{T} = \frac{\partial \Psi^e}{\partial \mathbf{E}}, \quad (9)$$

which are related by

$$\mathbf{T}^e = \mathbf{F}^p \cdot \mathbf{T} \cdot \mathbf{F}^{pT}. \quad (10)$$

The fourth-order elastic moduli tensors  $\mathcal{L}^e$  and  $\mathcal{L}$  are introduced by

$$\mathcal{L}^e = \frac{\partial^2 \Psi^e}{\partial \mathbf{E}^e \otimes \partial \mathbf{E}^e}, \quad \mathcal{L} = \frac{\partial^2 \Psi^e}{\partial \mathbf{E} \otimes \partial \mathbf{E}}. \quad (11)$$

Their rectangular components are related according to

$$\mathcal{L}_{ijkl} = F_{im}^{p-1} F_{jn}^{p-1} \mathcal{L}_{mnpq}^e F_{pk}^{p-T} F_{ql}^{p-T}. \quad (12)$$

Both tensors possess the full symmetry. The tensor  $\mathcal{L}^e$  appears in the linear relationship between the rates  $\dot{\mathbf{T}}^e$  and  $\dot{\mathbf{E}}^e$ , i.e.,

$$\dot{\mathbf{T}}^e = \mathcal{L}^e : \dot{\mathbf{E}}^e, \quad \dot{T}_{ij} = \mathcal{L}_{ijkl}^e \dot{E}_{kl}, \quad (13)$$

which follows by differentiating the first expression in Eq. (9). A differentiation of Eq. (10) gives

$$\dot{\mathbf{T}}^e = \mathbf{F}^p \cdot (\dot{\mathbf{T}} + \mathbf{Z}^p \cdot \mathbf{T} + \mathbf{T} \cdot \mathbf{Z}^{pT}) \cdot \mathbf{F}^{pT}, \quad (14)$$

where the second-order tensor  $\mathbf{Z}^p$  is defined by

$$\mathbf{Z}^p = \mathbf{F}^{p-1} \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1}) \cdot \mathbf{F}^p. \quad (15)$$

Since, from Eq. (6),

$$\dot{\mathbf{E}}^e = \mathbf{F}^{p-T} \cdot \{\dot{\mathbf{E}} - \mathbf{F}^{pT} \cdot [\mathbf{C}^e \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1})]_s \cdot \mathbf{F}^p\} \cdot \mathbf{F}^{p-1}, \quad (16)$$

the substitution of Eqs. (14) and (16) into Eq. (13) yields

$$\dot{\mathbf{T}} = \mathcal{L} : \{\dot{\mathbf{E}} - \mathbf{F}^{pT} \cdot [\mathbf{C}^e \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1})]_s \cdot \mathbf{F}^p\} - (\mathbf{Z}^p \cdot \mathbf{T} + \mathbf{T} \cdot \mathbf{Z}^{pT}). \quad (17)$$

The elastic part of the rate of Lagrangian strain is defined by Hill and Rice (1973) as

$$(\dot{\mathbf{E}})^e = \mathcal{L}^{-1} : \dot{\mathbf{T}}. \quad (18)$$

This is associated with a reversible strain increment in an infinitesimal loading/unloading stress cycle corresponding to  $\dot{\mathbf{T}}$ . The remaining part of the strain rate in the additive partition

$$\dot{\mathbf{E}} = (\dot{\mathbf{E}})^e + (\dot{\mathbf{E}})^p, \quad (19)$$

is the plastic part  $(\dot{\mathbf{E}})^p$ , which gives rise to a residual strain increment left upon the considered infinitesimal loading/unloading stress cycle. If material obeys the Ilyushin's postulate, Hill and Rice have shown that  $(\dot{\mathbf{E}})^p$  so defined is codirectional with the outward normal to a locally smooth yield surface in the stress  $\mathbf{T}$  space.

Note that it is the tensor  $\mathcal{L}^{-1}$  and not  $\mathcal{L}^{e-1}$  that appears in the definition of elastic part of the strain rate (18). This should be compared with Eq. (13), which indicates that  $\mathcal{L}^{e-1}$  and  $\dot{\mathbf{T}}^e$  appear in the definition of  $\dot{\mathbf{E}}^e$ , i.e.,

$$\dot{\mathbf{E}}^e = \mathcal{L}^{e-1} : \dot{\mathbf{T}}^e. \quad (20)$$

In general, the two rates are different, i.e.,  $(\dot{\mathbf{E}})^e \neq \dot{\mathbf{E}}^e$ . Likewise,  $(\dot{\mathbf{E}})^p = \dot{\mathbf{E}} - (\dot{\mathbf{E}})^e \neq \dot{\mathbf{E}}^p$ . While  $(\dot{\mathbf{E}})^e$  and  $(\dot{\mathbf{E}})^p$  sum up to give  $\dot{\mathbf{E}}$ , in general  $\dot{\mathbf{E}}^e + \dot{\mathbf{E}}^p \neq \dot{\mathbf{E}}$ .

The relationships between the constituents of the multiplicative decomposition (1) and the additive decomposition (19) follow from Eq. (17). The plastic part of the rate of Lagrangian strain can be written as

$$(\dot{\mathbf{E}})^p = \mathbf{F}^{pT} \cdot [\mathbf{C}^e \cdot (\dot{\mathbf{F}}^p \cdot \mathbf{F}^{p-1})]_s \cdot \mathbf{F}^p + \mathcal{L}^{-1} : (\mathbf{Z}^p \cdot \mathbf{T} + \mathbf{T} \cdot \mathbf{Z}^{pT}). \quad (21)$$

The elastic part  $(\dot{\mathbf{E}})^e$  is related to  $\dot{\mathbf{E}}^e$  by

$$(\dot{\mathbf{E}})^e = \mathbf{F}^{pT} \cdot \dot{\mathbf{E}}^e \cdot \mathbf{F}^p - \mathcal{L}^{-1} : (\mathbf{Z}^p \cdot \mathbf{T} + \mathbf{T} \cdot \mathbf{Z}^{pT}), \quad (22)$$

where

$$\dot{\mathbf{E}}^e = \mathbf{F}^{eT} \cdot (\dot{\mathbf{F}}^e \cdot \mathbf{F}^{e-1})_s \cdot \mathbf{F}^e. \quad (23)$$

Dually to previous formulation, the elastic part of the rate of symmetric Piola–Kirchhoff stress is defined by

$$(\dot{\mathbf{T}})^e = \mathcal{L} : \dot{\mathbf{E}}. \quad (24)$$

The remaining part,

$$(\dot{\mathbf{T}})^p = \dot{\mathbf{T}} - \mathcal{L} : \dot{\mathbf{E}}, \quad (25)$$

is the plastic part of the stress rate, which is codirectional with the inward normal to a locally smooth yield surface in the strain  $\mathbf{E}$  space. The relationships between plastic parts of the stress and strain rates are (Hill, 1978)

$$(\dot{\mathbf{T}})^p = -\mathcal{L} : (\dot{\mathbf{E}})^p, \quad (\dot{\mathbf{E}})^p = -\mathcal{L}^{-1} : (\dot{\mathbf{T}})^p. \quad (26)$$

### 3. Partitioning of the rate of deformation gradient

The previous analysis can be extended to partition the rate of deformation gradient into its elastic and plastic parts, such that

$$\dot{\mathbf{F}} = (\dot{\mathbf{F}})^e + (\dot{\mathbf{F}})^p. \quad (27)$$

To that goal, we first note that the nonsymmetric nominal stress tensors  $\mathbf{P}^e = \mathbf{T}^e \cdot \mathbf{F}^{eT}$  and  $\mathbf{P} = \mathbf{T} \cdot \mathbf{F}^T$  can be derived from the elastic strain energy  $\Psi^e$  by the gradient operations

$$\mathbf{P}^e = \frac{\partial \Psi^e}{\partial \mathbf{F}^e}, \quad \mathbf{P} = \frac{\partial \Psi^e}{\partial \mathbf{F}}, \quad (28)$$

such that

$$\mathbf{P}^e = \mathbf{F}^p \cdot \mathbf{P}. \quad (29)$$

The fourth-order elastic pseudomoduli tensors are introduced by

$$\mathbf{\Lambda}^e = \frac{\partial^2 \Psi^e}{\partial \mathbf{F}^e \otimes \partial \mathbf{F}^e}, \quad A_{ijkl}^e = \frac{\partial^2 \Psi^e}{\partial F_{ji}^e \partial F_{lk}^e}, \quad (30)$$

$$\mathbf{\Lambda} = \frac{\partial^2 \Psi^e}{\partial \mathbf{F} \otimes \partial \mathbf{F}}, \quad A_{ijkl} = \frac{\partial^2 \Psi^e}{\partial F_{ji} \partial F_{lk}}. \quad (31)$$

It can be easily verified by partial differentiation that the rectangular components of the two pseudomoduli tensors are related through

$$A_{ijkl}^e = F_{im}^p A_{mjnl} F_{kn}^p. \quad (32)$$

The pseudomoduli tensors do not possess the symmetry in the leading or terminal pair of indices, but do possess the reciprocal symmetry ( $A_{ijkl}^e = A_{klij}^e$  and  $A_{ijkl} = A_{klij}$ ). The pseudomoduli tensor  $\mathbf{\Lambda}^e$  appears in the linear relationship between the rates  $\dot{\mathbf{P}}^e$  and  $\dot{\mathbf{F}}^e$ , such that

$$\dot{\mathbf{P}}^e = \mathbf{\Lambda}^e \cdot \dot{\mathbf{F}}^e, \quad \dot{P}_{ij}^e = A_{ijkl}^e \dot{F}_{lk}^e. \quad (33)$$

This follows by differentiating the first of the expressions in Eq. (28). On the other hand, a differentiation of Eq. (29) gives

$$\dot{\mathbf{P}}^e = \mathbf{F}^p \cdot \dot{\mathbf{P}} + \dot{\mathbf{F}}^p \cdot \mathbf{P}. \quad (34)$$

Substitution of Eqs. (34) and (32) into Eq. (33) yields

$$\dot{\mathbf{P}} = \mathbf{\Lambda} \cdot \cdot (\dot{\mathbf{F}}^e \cdot \mathbf{F}^p) - \mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{P}. \quad (35)$$

Furthermore, from the multiplicative decomposition (1), the rate of deformation gradient is

$$\dot{\mathbf{F}} = \dot{\mathbf{F}}^e \cdot \mathbf{F}^p + \mathbf{F}^e \cdot \dot{\mathbf{F}}^p. \quad (36)$$

Consequently, Eq. (35) can be rewritten as

$$\dot{\mathbf{P}} = \mathbf{\Lambda} \cdot \cdot (\dot{\mathbf{F}} - \mathbf{F}^e \cdot \dot{\mathbf{F}}^p) - \mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{P}, \quad (37)$$

or,

$$\dot{\mathbf{P}} = \mathbf{\Lambda} \cdot \cdot [\dot{\mathbf{F}} - \mathbf{F}^e \cdot \dot{\mathbf{F}}^p - \mathbf{\Lambda}^{-1} \cdot \cdot (\mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{P})]. \quad (38)$$

The elastic part of the rate of deformation gradient is defined by

$$(\dot{\mathbf{F}})^e = \mathbf{\Lambda}^{-1} \cdot \cdot \dot{\mathbf{P}}. \quad (39)$$

It is assumed that the elastic pseudomoduli tensor  $\mathbf{\Lambda}$  has its inverse, the elastic pseudocompliances tensor  $\mathbf{\Lambda}^{-1}$ , such that

$$\mathbf{\Lambda} \cdot \cdot \mathbf{\Lambda}^{-1} = \mathbf{\Lambda}^{-1} \cdot \cdot \mathbf{\Lambda} = \mathbf{I}. \quad (40)$$

When the components of  $\mathbf{\Lambda}$  and  $\mathbf{\Lambda}^{-1}$  are expressed in the same rectangular coordinate system,  $I_{ijkl} = \delta_{ij} \delta_{jk}$  and  $A_{ijmn} A_{nmkl} = I_{ijkl}$ . The remaining part of the rate of deformation gradient in Eq. (27),  $(\dot{\mathbf{F}})^p = \dot{\mathbf{F}} - (\dot{\mathbf{F}})^e$ , is codirectional with the outward normal to a locally smooth yield surface in the stress  $\mathbf{P}$  space. This normality is further discussed in Section 4.

The relationships between the constituents of the multiplicative decomposition (1) and the additive decomposition (27) follow from Eq. (38). They are

$$(\dot{\mathbf{F}})^p = \mathbf{F}^e \cdot \dot{\mathbf{F}}^p + \mathbf{\Lambda}^{-1} \cdot \cdot (\mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{P}), \quad (41)$$

$$(\dot{\mathbf{F}})^e = \dot{\mathbf{F}}^e \cdot \mathbf{F}^p - \mathbf{\Lambda}^{-1} \cdot \cdot (\mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{P}). \quad (42)$$

It is noted that under the superposed rotations of the current and intermediate configurations, the nominal stress tensors  $\mathbf{P}$  and  $\mathbf{P}^e$  change according to  $\mathbf{P}^* = \mathbf{P} \cdot \mathbf{Q}^T$  and  $\mathbf{P}^{e*} = \hat{\mathbf{Q}} \cdot \mathbf{P}^e \cdot \mathbf{Q}^T$ . However, neither  $\dot{\mathbf{F}}$ , nor  $(\dot{\mathbf{F}})^e$  or  $(\dot{\mathbf{F}})^p$ , depends on the rotation of the intermediate configuration  $\hat{\mathbf{Q}}$ .

Eq. (38) also serves to identify the elastic and plastic parts of the rate of nominal stress. These are

$$(\dot{\mathbf{P}})^e = \mathbf{\Lambda} \cdot \cdot \dot{\mathbf{F}}, \quad (43)$$

$$(\dot{\mathbf{P}})^p = -[\mathbf{F}^{p-1} \cdot \dot{\mathbf{F}}^p \cdot \mathbf{P} + \mathbf{\Lambda} \cdot \cdot (\mathbf{F}^e \cdot \dot{\mathbf{F}}^p)], \quad (44)$$

such that

$$\dot{\mathbf{P}} = (\dot{\mathbf{P}})^e + (\dot{\mathbf{P}})^p. \quad (45)$$

By comparing Eqs. (41) and (44), the plastic parts of the rate of nominal stress and deformation gradient are related by

$$(\dot{\mathbf{P}})^p = -\mathbf{\Lambda} \cdot \cdot (\dot{\mathbf{F}})^p, \quad (\dot{\mathbf{F}})^p = -\mathbf{\Lambda}^{-1} \cdot \cdot (\dot{\mathbf{P}})^p. \quad (46)$$

### 3.1. Relationship between $(\dot{\mathbf{P}})^p$ and $(\dot{\mathbf{T}})^p$

To derive the relationship between plastic parts of the rate of nominal and symmetric Piola–Kirchhoff stress,

$$(\dot{\mathbf{P}})^p = \dot{\mathbf{P}} - \mathbf{\Lambda} \cdot \cdot \dot{\mathbf{F}}, \quad (\dot{\mathbf{T}})^p = \dot{\mathbf{T}} - \mathcal{L} : \dot{\mathbf{E}}, \quad (47)$$

we first recall the relationships between  $\dot{\mathbf{P}}$  and  $\dot{\mathbf{T}}$ , and  $\mathbf{\Lambda}$  and  $\mathcal{L}$ . Following Hill (1984) and Havner (1992), these can be conveniently written as

$$\mathbf{\Lambda} = \mathcal{K}^T : \mathcal{L} : \mathcal{K} + \mathcal{T}, \quad \dot{\mathbf{P}} = \mathcal{K}^T : \dot{\mathbf{T}} + \mathcal{T} \cdot \cdot \dot{\mathbf{F}}. \quad (48)$$

The rectangular components of the fourth-order tensors  $\mathcal{K}$  and  $\mathcal{T}$  are

$$\mathcal{K}_{ijkl} = \frac{1}{2}(\delta_{ik}F_{lj} + \delta_{jk}F_{li}), \quad \mathcal{T}_{ijkl} = T_{ik}\delta_{jl}. \quad (49)$$

The relationship between  $(\dot{\mathbf{P}})^p$  and  $(\dot{\mathbf{T}})^p$  is obtained by taking the trace product of the second equation in Eq. (47) with  $\mathcal{K}^T$  from the left. Upon using Eq. (48), this yields (Hill, 1984)

$$(\dot{\mathbf{P}})^p = \mathcal{K}^T : (\dot{\mathbf{T}})^p. \quad (50)$$

Since

$$(\dot{\mathbf{P}})^p = -\mathbf{\Lambda} \cdot \cdot (\dot{\mathbf{F}})^p, \quad (\dot{\mathbf{T}})^p = -\mathcal{L} : (\dot{\mathbf{E}})^p, \quad (51)$$

the plastic parts of the rates of the deformation gradient and the Lagrangian strain are related by

$$(\dot{\mathbf{F}})^p = \mathbf{\Lambda}^{-1} \cdot \cdot \mathcal{K}^T : \mathcal{L} : (\dot{\mathbf{E}})^p. \quad (52)$$

In addition, it is noted that

$$\dot{\mathbf{F}} \cdot \cdot (\dot{\mathbf{P}})^p = \dot{\mathbf{E}} : (\dot{\mathbf{T}})^p, \quad (53)$$

which follows by taking the trace product of Eq. (50) with  $\dot{\mathbf{F}}$  from the left, and by using  $\mathcal{K} \cdot \cdot \dot{\mathbf{F}} = \dot{\mathbf{F}} \cdot \cdot \mathcal{K}^T = \dot{\mathbf{E}}$ .

#### 4. Normality properties

The last expression is particularly helpful to discuss the plastic normality rules. This can be done by using the framework of Hill and Rice (1973) and Hill (1978). If increments rather than rates are used, we can rewrite Eq. (53) as

$$d\mathbf{F} \cdot d^p\mathbf{P} = d\mathbf{E} : d^p\mathbf{T}. \quad (54)$$

An analogous expression holds when increments of  $\mathbf{F}$  and  $\mathbf{E}$  along an unloading elastic branch of the response are used, i.e.,

$$\delta\mathbf{F} \cdot d^p\mathbf{P} = \delta\mathbf{E} : d^p\mathbf{T}. \quad (55)$$

If this is positive, the material complies with the normality rule in the deformation space. Plastic increment  $d^p\mathbf{P}$  is then codirectional with the inward normal to a locally smooth yield surface  $g(\mathbf{F}, \mathcal{H}) = 0$  in the deformation gradient space, such that

$$d^p\mathbf{P} = -d\gamma \frac{\partial g}{\partial \mathbf{F}}. \quad (56)$$

The inelastic history-dependent parameters are collectively denoted by  $\mathcal{H}$ , and  $d\gamma$  is the loading index. Since

$$d^p\mathbf{P} = -\mathbf{A} \cdot d^p\mathbf{F}, \quad d^p\mathbf{T} = -\mathcal{L} : d^p\mathbf{E}, \quad (57)$$

and

$$\delta\mathbf{P} = \mathbf{A} \cdot \delta\mathbf{F}, \quad \delta\mathbf{T} = \mathcal{L} : \delta\mathbf{E}, \quad (58)$$

the substitution into Eq. (55) yields a dual relationship

$$\delta\mathbf{P} \cdot d^p\mathbf{F} = \delta\mathbf{T} : d^p\mathbf{E}. \quad (59)$$

When this is negative, the material complies with the normality rule in the stress space. In that case, the plastic increment  $d^p\mathbf{F}$  is codirectional with the outward normal to a locally smooth yield surface  $f(\mathbf{P}, \mathcal{H}) = 0$  in the nominal stress space, i.e.,

$$d^p\mathbf{F} = d\gamma \frac{\partial f}{\partial \mathbf{P}}. \quad (60)$$

The yield surface normals in the deformation gradient and the nominal stress space are related by

$$\frac{\partial g}{\partial \mathbf{F}} = \frac{\partial f}{\partial \mathbf{P}} \cdot \mathbf{A}. \quad (61)$$

The loading index can be expressed as either of

$$d\gamma = \frac{1}{H} \frac{\partial f}{\partial \mathbf{P}} \cdot d^p\mathbf{P} = \frac{1}{h} \frac{\partial g}{\partial \mathbf{F}} \cdot d\mathbf{F} > 0. \quad (62)$$

The scalar parameters  $H$  and  $h$  are related by

$$H = h - \frac{\partial g}{\partial \mathbf{F}} \cdot \frac{\partial f}{\partial \mathbf{P}}. \quad (63)$$

A sufficient condition for the normality is the compliance with the Ilyushin's (1961) postulate of positive network in an isothermal cycle of strain that involves plastic deformation, since then the quantity in Eq. (54) must be negative (Hill and Rice, op. cit.), i.e.,

$$d\mathbf{F} \cdot d^p\mathbf{P} = d\mathbf{E} : d^p\mathbf{T} < 0. \quad (64)$$

On the other hand, Eq. (54) does not have a dual relationship, since

$$d\mathbf{P} \cdot \cdot d^p\mathbf{F} \neq d\mathbf{T} : d^p\mathbf{E}. \quad (65)$$

Instead, we can only write

$$d\mathbf{F} \cdot \cdot \mathbf{A} \cdot \cdot d^p\mathbf{F} = d\mathbf{E} : \mathcal{L} : d^p\mathbf{E}, \quad (66)$$

or

$$d\mathbf{P} \cdot \cdot d^p\mathbf{F} + d^p\mathbf{F} \cdot \cdot \mathbf{A} \cdot \cdot d^p\mathbf{F} = d\mathbf{T} : d^p\mathbf{E} + d^p\mathbf{E} : \mathcal{L} : d^p\mathbf{E}. \quad (67)$$

If material is in the hardening range relative to conjugate measures  $\mathbf{E}$  and  $\mathbf{T}$ , the stress increment  $d\mathbf{T}$ , producing plastic deformation  $d^p\mathbf{E}$ , is directed outside the yield surface in the stress  $\mathbf{T}$  space, satisfying  $d\mathbf{T} : d^p\mathbf{E} > 0$ . If material is in the softening range, the stress increment producing plastic deformation is directed inside the yield surface, satisfying the reversed inequality. As seen from Eq. (67), in each case the sign of  $d\mathbf{P} \cdot \cdot d^p\mathbf{F}$  is not determined by the sign of  $d\mathbf{T} \cdot \cdot d^p\mathbf{E}$  alone.

## 5. Monocrystalline plasticity

Suppose that crystallographic slip is the only mechanism of plastic deformation in a single crystal, and consider plastic deformation to occur by smooth shearing on the slip planes and in the slip directions. The deformation gradient in this model can be decomposed as in Eq. (1), where  $\mathbf{F}^p$  is the part of  $\mathbf{F}$  due to slip only, while  $\mathbf{F}^e$  is the part due to lattice stretching and rotation. Denote the unit vector in the slip direction and the unit normal to the corresponding slip plane in the undeformed configuration by  $\mathbf{s}_0^\alpha$  and  $\mathbf{m}_0^\alpha$ , where  $\alpha$  designates the slip system. The vector  $\mathbf{s}_0^\alpha$  is embedded in the lattice, so that it becomes  $\mathbf{s}^\alpha = \mathbf{F}^e \cdot \mathbf{s}_0^\alpha$  in the deformed configuration. The normal to the slip plane in the deformed configuration is defined by the reciprocal vector  $\mathbf{m}^\alpha = \mathbf{m}_0^\alpha \cdot \mathbf{F}^{e-1}$ . In general,  $\mathbf{s}^\alpha$  and  $\mathbf{m}^\alpha$  are not unit vectors, but are orthogonal to each other.

The rate of plastic deformation gradient can be expressed in terms of the slip rates  $\dot{\gamma}^\alpha$  as

$$\dot{\mathbf{F}}^p = \sum_{\alpha=1}^n \dot{\gamma}^\alpha (\mathbf{s}_0^\alpha \otimes \mathbf{m}_0^\alpha) \cdot \mathbf{F}^p. \quad (68)$$

The number of momentarily active slip systems is  $n$ . Upon substitution into Eq. (41), the plastic part of the rate of deformation gradient becomes

$$(\dot{\mathbf{F}})^p = \sum_{\alpha=1}^n \mathbf{A}^\alpha \dot{\gamma}^\alpha, \quad (69)$$

where

$$\mathbf{A}^\alpha = (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) \cdot \mathbf{F} + \mathbf{A}^{-1} \cdot \cdot \mathbf{F}^{-1} \cdot (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) \cdot \mathbf{F} \cdot \mathbf{P}. \quad (70)$$

The plastic part of the rate of nominal stress is then

$$(\dot{\mathbf{P}})^p = - \sum_{\alpha=1}^n \mathbf{B}^\alpha \dot{\gamma}^\alpha, \quad (71)$$

where

$$\mathbf{B}^\alpha = \mathbf{A} \cdot \cdot \mathbf{A}^\alpha = \mathbf{F}^{-1} \cdot (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) \cdot \mathbf{F} \cdot \mathbf{P} + \mathbf{A} \cdot \cdot (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) \cdot \mathbf{F}. \quad (72)$$

The rate of work per unit volume is

$$\mathbf{P} \cdot \dot{\mathbf{F}} = \mathbf{P} \cdot \cdot (\dot{\mathbf{F}}^e \cdot \mathbf{F}^p + \mathbf{F}^e \cdot \dot{\mathbf{F}}^p), \quad (73)$$

from which we identify the rate of slip work



$$\sum_{\alpha=1}^n \tau^{\alpha} \dot{\gamma}^{\alpha} = \mathbf{P} \cdot \cdot (\mathbf{F}^c \cdot \dot{\mathbf{F}}^p). \quad (74)$$

The generalized resolved shear stress on the slip system  $\alpha$  is denoted by  $\tau^{\alpha}$ . Substituting Eq. (68) for  $\dot{\mathbf{F}}^p$  gives

$$\sum_{\alpha=1}^n \tau^{\alpha} \dot{\gamma}^{\alpha} = \mathbf{P} \cdot \cdot \sum_{\alpha=1}^n \mathbf{F}^c \cdot (\mathbf{s}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}) \cdot \mathbf{F}^p \dot{\gamma}^{\alpha}. \quad (75)$$

Thus, the generalized resolved shear stress can be expressed in terms of the nominal stress  $\mathbf{P}$  as

$$\tau^{\alpha} = \mathbf{P} \cdot \cdot [\mathbf{F} \cdot \mathbf{F}^{p-1} \cdot (\mathbf{s}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}) \cdot \mathbf{F}^p]. \quad (76)$$

The direction of the normal to the yield plane  $\tau^{\alpha} = \tau_{cr}^{\alpha}$  at  $\mathbf{P}$  is determined from the gradient  $\partial \tau^{\alpha} / \partial \mathbf{P}$ . This is, from Eq. (76),

$$\frac{\partial \tau^{\alpha}}{\partial \mathbf{P}} = \mathbf{F} \cdot \mathbf{F}^{p-1} \cdot (\mathbf{s}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}) \cdot \mathbf{F}^p + \mathbf{A}^{-1} \cdot \cdot [\mathbf{F}^{p-1} \cdot (\mathbf{s}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}) \cdot \mathbf{F}^p \cdot \mathbf{P}], \quad (77)$$

or

$$\frac{\partial \tau^{\alpha}}{\partial \mathbf{P}} = (\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}) \cdot \mathbf{F} + \mathbf{A}^{-1} \cdot \cdot \mathbf{F}^{-1} \cdot (\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}) \cdot \mathbf{F} \cdot \mathbf{P}. \quad (78)$$

The right-hand side is equal to  $\mathbf{A}^{\alpha}$  in Eq. (70) and, therefore,

$$\frac{\partial \tau^{\alpha}}{\partial \mathbf{P}} = \mathbf{A}^{\alpha}. \quad (79)$$

In view of Eq. (69), this establishes the normality property for the plastic part of the rate of deformation gradient,

$$(\dot{\mathbf{F}})^p = \sum_{\alpha=1}^n \frac{\partial \tau^{\alpha}}{\partial \mathbf{P}} \dot{\gamma}^{\alpha}. \quad (80)$$

Dually, by taking the gradient of Eq. (76) with respect to  $\mathbf{F}$ , there follows

$$\frac{\partial \tau^{\alpha}}{\partial \mathbf{F}} = \mathbf{A} \cdot \cdot [\mathbf{F} \cdot \mathbf{F}^{p-1} \cdot (\mathbf{s}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}) \cdot \mathbf{F}^p] + \mathbf{F}^{p-1} \cdot (\mathbf{s}_0^{\alpha} \otimes \mathbf{m}_0^{\alpha}) \cdot \mathbf{F}^p \cdot \mathbf{P}. \quad (81)$$

The right-hand side is equal to  $\mathbf{B}^{\alpha}$  in Eq. (72). In view of Eq. (71), this leads to normality property for plastic part of the rate of nominal stress

$$(\dot{\mathbf{P}})^p = - \sum_{\alpha=1}^n \frac{\partial \tau^{\alpha}}{\partial \mathbf{F}} \dot{\gamma}^{\alpha}. \quad (82)$$

Eqs. (80) and (82) are in agreement with Eqs. (6.19) and (6.20) of Havner (1992), since they can be rewritten as

$$(\dot{\mathbf{F}})^p = \frac{\partial}{\partial \mathbf{P}} \sum_{\alpha=1}^n (\tau^{\alpha} \dot{\gamma}^{\alpha}), \quad (\dot{\mathbf{P}})^p = - \frac{\partial}{\partial \mathbf{F}} \sum_{\alpha=1}^n (\tau^{\alpha} \dot{\gamma}^{\alpha}), \quad (83)$$

with the understanding that partial differentiations are performed at fixed  $\dot{\gamma}^{\alpha}$ . This implies that  $\sum (\tau^{\alpha} \dot{\gamma}^{\alpha})$  acts as the plastic potential for  $(\dot{\mathbf{F}})^p$  over an elastic domain in  $\mathbf{P}$  space, while  $-\sum (\tau^{\alpha} \dot{\gamma}^{\alpha})$  acts as the plastic potential for  $(\dot{\mathbf{P}})^p$  over an elastic domain in  $\mathbf{F}$  space.

## Acknowledgements

Research funding provided by the Los Alamos National Laboratories is kindly acknowledged. We also thank the reviewers for their comments and suggestions.

## References

- Havner, K.S., 1992. *Finite Plastic Deformation of Crystalline Solids*. Cambridge University Press, Cambridge.
- Hill, R., 1978. Aspects of invariance in solid mechanics. *Adv. Appl. Mech.* 18, 1–75.
- Hill, R., 1984. On macroscopic effects of heterogeneity in elastoplastic media at finite strain. *Math. Proc. Camb. Phil. Soc.* 95, 481–494.
- Hill, R., Rice, J.R., 1973. Elastic potentials and the structure of inelastic constitutive laws. *SIAM J. Appl. Math.* 25, 448–461.
- Ilyushin, A.A., 1961. On the postulate of plasticity. *Prikl. Math. Mekh.* 25, 503–507.
- Lee, E.H., 1969. Elastic–plastic deformation at finite strains. *J. Appl. Mech.* 36, 1–6.
- Lubarda, V.A., 1991. Constitutive analysis of large elasto-plastic deformation based on the multiplicative decomposition of deformation gradient. *Int. J. Solids Struct.* 27, 885–895.
- Lubarda, V.A., 1994. Elastoplastic constitutive analysis with the yield surface in strain space. *J. Mech. Phys. Solids* 42, 931–952.
- Lubarda, V.A., Lee, E.H., 1981. A correct definition of elastic and plastic deformation and its computational significance. *J. Appl. Mech.* 48, 35–40.
- Mandel, J., 1973. Equations constitutives et directeurs dans les milieux plastiques et viscoplastiques. *Int. J. Solids Struct.* 9, 725–740.
- Naghdi, P.M., 1990. A critical review of the state of finite plasticity. *Z. angew. Math. Phys.* 41, 315–394.
- Simo, J.C., Hughes, T.J.R., 1998. *Computational Inelasticity*. Springer, New York.