Boundary conditions in small-deformation, single-crystal plasticity that account for the Burgers vector

Morton E. Gurtin[‡] and Alan Needleman[†]

[‡]Department of Mathematical Sciences
Carnegie Mellon University
Pittsburgh, PA 15213, USA

[†]Division of Engineering
Brown University
Providence, RI 02912, USA

Abstract

This paper discusses boundary conditions appropriate to a theory of single-crystal plasticity (Gurtin, 2002) that includes an accounting for the Burgers vector through energetic and dissipative dependences on the tensor $\mathbf{G} = \operatorname{curl}\mathbf{H}^p$, with $\mathbf{H}^p$ the plastic part in the additive decomposition of the displacement gradient into elastic and plastic parts. This theory results in a flow rule in the form of N coupled second-order partial differential equations for the slip-rates $\dot\gamma^\alpha$ ($\alpha = 1, 2 \ldots, N$), and, consequently, requires higher-order boundary conditions. Motivated by the virtual-power principle in which the external power contains a boundary-integral linear in the slip-rates, *hard-slip conditions* in which

(A) $\dot\gamma^\alpha = 0$ on a subsurface $\mathcal{S}_{\mathrm{hard}}$ of the boundary

for all slip systems α are proposed. In this paper we develop a theory that is consistent with that of (Gurtin, 2002), but that leads to an external power containing a boundary-integral linear in the tensor $\dot H^p_{ij}\varepsilon_{jrl}n_r$, a result that motivates replacing (A) with the *microhard condition*

(B) $\dot H^p_{ij}\varepsilon_{jrl}n_r = 0$ on the subsurface $\mathcal{S}_{\mathrm{hard}}$.

We show that, interestingly, (B) may be interpreted as the requirement that there be no flow of the Burgers vector across $\mathcal{S}_{\mathrm{hard}}$.

What is most important, we establish uniqueness for the underlying initial/boundary-value problem associated with (B); since the conditions (A) are generally stronger than the conditions (B), this result indicates lack of existence for problems based on (A). For that reason, the hard-slip conditions (A) would seem inappropriate as boundary conditions.

Finally, we discuss conditions at a grain boundary based on the flow of the Burgers vector at and across the boundary surface.

Keywords: A. Dislocations; C. Crystal plasticity; D. Non-local plasticity

1 Introduction

We work within the framework of small deformations, neglecting geometric changes.

Let $\mathbf{u}(\mathbf{x}, t)$ denote the displacement of an arbitrary point $\mathbf{x}$ in B, the region of space occupied by the body. We base our discussion on the standard decomposition

$$\nabla\mathbf{u} = \mathbf{H}^e + \mathbf{H}^p, \tag{1.1}$$

in which $\mathbf{H}^e$ represents stretching and rotation of the *lattice*, while $\mathbf{H}^p$, the *plastic distortion*, represents local deformation due to slip. The symmetric part of $\mathbf{H}^e$, namely

$$\mathbf{E}^e = \tfrac{1}{2}(\mathbf{H}^e + \mathbf{H}^{e\top}), \tag{1.2}$$

is the *lattice strain.*

Single-crystal plasticity is based on the hypothesis that plastic flow take place through slip on prescribed slip systems $\alpha = 1, 2, \ldots, N$, with each system α defined by a *slip direction* $\mathbf{s}^\alpha$ and a *slip-plane normal* $\mathbf{m}^\alpha$, where

$$\mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0, \qquad |\mathbf{s}^\alpha|, |\mathbf{m}^\alpha| = 1, \qquad \mathbf{s}^\alpha, \mathbf{m}^\alpha = \text{constant.} \tag{1.3}$$

This hypothesis manifests itself in the requirement that $\mathbf{H}^p$ be characterized by *slips* (microshears) $\gamma^\alpha(\mathbf{x}, t)$ on the individual slip systems via the *kinematical constitutive assumption*

$$\mathbf{H}^p = \sum_\alpha \gamma^\alpha \, \mathbb{S}^\alpha, \tag{1.4}$$

with

$$\mathbb{S}^\alpha = \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \tag{1.5}$$

the *Schmid tensor* for α. Here and in what follows, lower case Greek superscripts $\alpha, \beta, \ldots$ denote slip-system labels and as such have the range $1, 2, \ldots, N$.

Recently, Gurtin (2002)[1] developed a gradient theory of single-crystal plasticity that accounts for the Burgers vector[2] as characterized by the field

$$\mathbf{G} = \operatorname{curl} \mathbf{H}^p \qquad \left(G_{ij} = \epsilon_{irs} \frac{\partial G_{js}}{\partial x_r} \right).$$

Central to this theory is the introduction of a system of microforces whose working accompanies slip as described by the slips γ^α; specifically, the microforce system consists of *vector* stresses $\boldsymbol{\xi}^\alpha$ and *scalar* internal forces π^α whose power expenditure, within any part R of the body B, is given by

$$\sum_\alpha \int_R (\pi^\alpha \dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \operatorname{grad} \dot{\gamma}^\alpha) \, dV. \tag{1.6}$$

This theoretical structure leads — via the principle of virtual power in conjunction with thermodynamically admissible constitutive equations based on a free energy dependent on $\mathbf{G}$ —

($\ddagger$) to a flow rule in the form of N coupled second-order partial differential equations for the slips

and to the microscopic external power-expenditure

$$\sum_\alpha \int_{\partial R} (\boldsymbol{\xi}^\alpha \cdot \mathbf{n}) \dot{\gamma}^\alpha \, dA. \tag{1.7}$$

Here $\mathbf{n}$ is the outward unit normal to ∂R.

Because of ($\ddagger$), microscopic boundary conditions are needed over and above the standard conditions for the macroscopic fields. Here, following (G-2002), we limit our discussion to two types of conditions:

(i) *microscopically hard boundary conditions* meant to characterize, for example, microscopic behavior at the boundary of a ductile metal perfectly bonded to a ceramic;

(ii) *microscopically free boundary conditions* meant to characterize microscopic behavior at a boundary whose environment exerts no microscopic forces on the body.

---

[1] Henceforth referred to as (G-2002).

[2] We refrain from using the term geometrically necessary dislocations, which we believe to be misleading in a continuum theory. The sensitivity of single-crystal plasticity to the local Burgers vector at small length scales is clear from the discrete-dislocation simulations of Cleverlinga, Van der Giessen, and Needleman (1999).

Based on (1.7) with $R = B$, boundary conditions for microscopically hard and microscopically free portions of ∂B are introduced in (G-2002); for the former the *hard-slip conditions*

$$\dot{\gamma}^\alpha = 0 \qquad \text{for all } \alpha \tag{1.8}$$

are proposed, while

$$\boldsymbol{\xi}^\alpha \cdot \mathbf{n} = 0 \qquad \text{for all } \alpha \tag{1.9}$$

are considered for the latter. Because of the transparent nature of the hard-slip conditions and because of (‡), the hard-slip conditions would, at first sight, seem a reasonable mathematical characterization of a microscopically hard boundary.

While gradient dependences are introduced in (G-2002) through a free energy dependent on $\mathbf{G}$, the framework itself applies equally well to more general dependences on slip gradients. This feature begs the question as to whether the Burgers tensor $\mathbf{G}$, since it represents a fundamental ingredient of the theory, could be introduced directly within the virtual-power framework. In this study we answer this question and in so doing arrive at an interesting and unexpected conclusion regarding the the hard-slip conditions (1.8).

To include the Burgers tensor $\mathbf{G}$ in the basic structure of the theory, we introduce a *defect stress* $\mathbb{T}$ that expends power over $\dot{\mathbf{G}}$ and replace the microscopic power expenditure (1.6) by

$$\int\limits_R \left(\mathbb{T} : \dot{\mathbf{G}} + \sum_\alpha \pi^\alpha \dot{\gamma}^\alpha \right) dV. \tag{1.10}$$

When combined with constitutive equations consistent with those of (G-2002), *this change results in exactly the same local equations within the body as those derived in* (G-2002), the two formulations being related by the expression

$$\boldsymbol{\xi}^\alpha = \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha \qquad (\xi_i^\alpha = \varepsilon_{ijk} m_j^\alpha \mathbb{T}_{kr} s_r^\alpha). \tag{1.11}$$

But the same cannot be said for the boundary conditions *suggested* by the two formulations.

The present study leads to an external microscopic power-expenditure

$$\underbrace{\int\limits_{\partial R} \left(\mathbb{T}^\top (\mathbf{n}\times) \right) : \dot{\mathbf{H}}^p \, dA}_{(\mathcal{L})} = -\underbrace{\int\limits_{\partial R} \mathbb{T}^\top \mathbb{P}(\mathbf{n}) : \left(\dot{\mathbf{H}}^p (\mathbf{n}\times) \right) dA}_{(\mathcal{R})}, \tag{1.12}$$

of which $(\mathcal{R})$ suggests a consideration of the *microhard condition*

$$\dot{\mathbf{H}}^p (\mathbf{n}\times) = \mathbf{0} \qquad (\dot{H}_{ij}^p \varepsilon_{jrl} n_r = 0). \tag{1.13}$$

On the other hand, virtual power applied to $(\mathcal{L})$ of (1.12) would require that the natural boundary condition be one that renders $(\mathcal{L})$ zero for any choice of $\dot{\mathbf{H}}^p$, and would therefore seem to suggest a mechanical boundary condition requiring that the deviatoric part of $\mathbb{T}^\top(\mathbf{n}\times)$ vanish. But, in light of (1.4), such a condition is implied by the vanishing of (L) only when the Schmid tensors $\mathbb{S}^\alpha = \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha$ span the space of deviatoric tensors.[3] More generally, in view of (1.4), the vanishing of (L) for any choice of slips suggests boundary conditions asserting that

$$\mathbb{S}^\alpha : \left(\mathbb{T}^\top(\mathbf{n}\times) \right) = 0 \qquad (\mathbb{S}_{ij}^\alpha \mathbb{T}_{ri} \varepsilon_{rkj} n_k = 0) \qquad \text{for all } \alpha. \tag{1.14}$$

The existence of two sets of boundary conditions — one set in terms of slip-rates $\dot{\gamma}^\alpha$ and microstresses $\boldsymbol{\xi}^\alpha \cdot \mathbf{n}$, the other in terms of the plastic distortion-rate $\dot{\mathbf{H}}^p$ and the defect stress $\mathbb{T}$ — and the form of the condition (1.13) lead to the following questions:

---

[3] *Cermelli's Theorem* (G-2002) asserts that for FCC and BCC crystals the N Schmid tensors $\mathbb{S}^\alpha$ span the space of deviatoric tensors. For such crystals *any deviatoric tensor* $\mathbf{H}^p$ *may be written in the form* (1.4). This result is clearly not true for HCP crystals, which have only four systems, or for any other crystal with less than 8 slip systems; for such crystals, the tensor space spanned by the Schmid tensors is not the space of deviatoric tensors, a restriction that we need bear in mind in what follows.

(i) Are the two sets of boundary conditions in any way related?

(ii) What is the physical meaning of the kinematical conditions (1.13)?

Regarding (i), it is not difficult to show, using (1.11), that $\mathbb{S}^{\alpha} \colon \big(\mathbb{T}^{\top}(\mathbf{n} \times)\big) = 0$ for all α if and only if $\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n} = 0$ for all α (Cermelli, 2003; private communication); thus the mechanical boundary conditions (1.9) and (1.14) are equivalent.

On the other hand, the hard-slip conditions (1.8) are generally *not* equivalent to the microhard condition (1.13). Indeed, by (1.4), (1.8) implies that $\dot{\mathbf{H}}^p = \mathbf{0}$, a condition stronger than $\dot{\mathbf{H}}^p(\mathbf{n} \times) = \mathbf{0}$. In §9 we establish *uniqueness* for the underlying boundary-value problem using the weaker condition $\dot{\mathbf{H}}^p(\mathbf{n} \times) = \mathbf{0}$. Thus one would expect lack of existence for this problem using the conditions (1.8). For that reason,

(†) *the hard-slip conditions* (1.8) *would seem inappropriate as boundary conditions.*[4]

To answer (ii) we note in §2.1 that $\mathbf{G}^{\top}\mathbf{e}$ provides a measure of the (local) Burgers vector for the plane with unit normal $\mathbf{e}$, and hence may be viewed as the local Burgers vector, per unit area, for those dislocation lines that pierce this plane (Burgers, 1939; Kröner, 1960). We show that, for any constant (unit) vector $\mathbf{e}$,

$$\overline{\dot{\mathbf{G}^{\top}\mathbf{e}}} = -\operatorname{div}\big(-\dot{\mathbf{H}}^p(\mathbf{e} \times)\big) \qquad \left(\overline{\dot{G_{ji}e_j}} = \frac{\partial}{\partial x_l}\Big(\dot{H}^p_{ij}\varepsilon_{jrl}e_r\Big)\right),$$

a balance that establishes $-\dot{\mathbf{H}}^p(\mathbf{e} \times)$ as a *Burgers-vector flux* and leads, after some analysis (cf. the argument leading to (2.17)), to the conclusion that $\dot{\mathbf{H}}^p(\mathbf{n} \times) = \mathbf{0}$ at a boundary point if and only if there is no flow of the Burgers vector across the boundary at that point. Thus the microscopically hard condition $\dot{\mathbf{H}}^p(\mathbf{n} \times) = \mathbf{0}$ has a precise physical meaning.

We close the paper by developing microscopic interface conditions at a *grain boundary* $\mathcal{G}$. These interface conditions are phrased in terms of the Burgers-vector flow across $\mathcal{S}$ and involve the fields $\dot{\mathbf{H}}^p(\mathbf{m} \times)$ and $\mathbb{T}^{\top}(\mathbf{m} \times)$, where $\mathbf{m}$ is the unit normal field for $\mathcal{G}$.[5] The resulting grain-boundary flow rules seem consistent with experiments of Sun et al. (1998, 2000), who determine the Burgers tensor in a bicrystal through measurements of lattice rotations.

---

[4] The simulations of Bittencourt, Needleman, Gurtin, and Van der Giessen (2002) and Nicola, Van der Geissen, and Needleman (2003) used the hard-slip conditions (1.8) with good result when discussing problems involving symmetric double slip, but in those special cases the "hard" boundary conditions (1.8) and (1.13) are equivalent. However, in the composite calculations of Bittencourt et al. (2003), which involved single slip, $\dot{\gamma}$ was taken to vanish on all matrix-particle interfaces, including those parallel to the slip direction. The considerations here indicate that $\dot{\gamma}$ should have been taken to vanish only on matrix-particle interfaces perpendicular to the slip direction (cf. the sentence containing (8.13)).

[5] Cf. Cermelli and Gurtin (2002) who, working within the framework of (G-2002), develop grain-boundary conditions conditions consisting of 2N relations between the slip-rates and microstresses at $\mathcal{G}$.

2   Macroscopic characterization of the Burgers vector

2.1   The Burgers tensor G

For **A** a tensor field,

$$(\operatorname{curl} \mathbf{A})_{ij} = \epsilon_{irs} \frac{\partial A_{js}}{\partial x_r},$$

with ϵ_{irs} the alternating symbol.

By Stokes' theorem, for $\mathcal{C}$ the boundary curve of a smooth oriented surface S with unit normal **e**,

$$\int_{\mathcal{C}} \mathbf{H}^p \, \mathbf{dx} = \int_S (\operatorname{curl} \mathbf{H}^p)^\top \mathbf{e} \, dA, \tag{2.1}$$

This integral is generally nonzero, as the plastic distortion $\mathbf{H}^p$ is not the gradient of a vector field, and we associate the vector measure $(\operatorname{curl} \mathbf{H}^p)^\top \mathbf{e} \, dA$ with the *Burgers vector* corresponding to the "boundary curve" of a surface-element $\mathbf{e} \, dA$. Thus, for

$$\mathbf{G} = \operatorname{curl} \mathbf{H}^p, \tag{2.2}$$

$\mathbf{G}^\top \mathbf{e}$ provides a measure of the (local) Burgers vector for the plane Π with unit normal **e**. We refer to **G** as the *Burgers tensor* and to $\mathbf{G}^\top \mathbf{e}$ *as the Burgers vector associated with small loops on* Π, it being understood that this Burgers vector is measured per unit area. Since

$$\big(\operatorname{curl}(\gamma^\alpha \, \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\big)_{ij} = \varepsilon_{irq} \frac{\partial \gamma^\alpha}{\partial x_r} s_j^\alpha m_q^\alpha = \big((\nabla \gamma^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{s}^\alpha\big)_{ij},$$

(1.4) yields (Fleck, Muller, Ashby, Hutchinson, 1994)

$$\mathbf{G} = \sum_\alpha (\nabla \gamma^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{s}^\alpha \qquad \left(G_{ij} = \sum_\alpha \left(\varepsilon_{irq} \frac{\partial \gamma^\alpha}{\partial x_r} m_q^\alpha s_j^\alpha \right) \right). \tag{2.3}$$

2.2   The tensor (a×) and the projection $\mathbb{P}(\mathbf{e})$

The following notation and terminology is useful in discussing the evolution of the Burgers vector. Given any vector **a**, we write $(\mathbf{a}\times)$ for the *tensor* defined by

$$(\mathbf{a}\times)_{ij} = \varepsilon_{ikj} a_k;$$

then

$$(\mathbf{a}\times)^\top = -(\mathbf{a}\times) \tag{2.4}$$

and

$$(\mathbf{a}\times)(\mathbf{b} \otimes \mathbf{c}) = (\mathbf{a} \times \mathbf{b}) \otimes \mathbf{c}, \qquad (\mathbf{b} \otimes \mathbf{c})(\mathbf{a}\times) = \mathbf{b} \otimes (\mathbf{c} \times \mathbf{a}). \tag{2.5}$$

For **e** a unit vector, we write

$$\mathbb{P}(\mathbf{e}) = \mathbf{1} - \mathbf{e} \otimes \mathbf{e}, \qquad P_{ij}(\mathbf{e}) = \delta_{ij} - e_i e_j, \tag{2.6}$$

for the *projection onto the plane perpendicular to* **e**. We then have the following identities:

$$(\mathbf{e}\times)\mathbb{P}(\mathbf{e}) = \mathbb{P}(\mathbf{e})(\mathbf{e}\times) = (\mathbf{e}\times), \qquad (\mathbf{e}\times)(\mathbf{e}\times) = -\mathbb{P}(\mathbf{e}), \qquad \mathbb{P}(\mathbf{e}) = \mathbb{P}(\mathbf{e})^\top. \tag{2.7}$$

By (2.5), $(\mathbf{e}\times)(\mathbf{e} \otimes \mathbf{e}) = (\mathbf{e} \otimes \mathbf{e})(\mathbf{e}\times) = \mathbf{0}$, which implies $(2.7)_1$; $(2.7)_2$ is easily verified using components and the identity $\varepsilon_{ijk}\varepsilon_{ipq} = \delta_{jp}\delta_{kq} - \delta_{jq}\delta_{kp}$.

Given any pair of tensors **A** and **B**, we have the *transfer identities*:

$$\big(\mathbf{A}(\mathbf{e}\times)\big) : \mathbf{B} = -\mathbf{A} : \big(\mathbf{B}(\mathbf{e}\times)\big), \tag{2.8}$$

$$= -\big(\mathbf{A}\mathbb{P}(\mathbf{e})\big) : \big(\mathbf{B}(\mathbf{e}\times)\big). \tag{2.9}$$

The first of these identities follows from (2.4). To prove the second, note that by $(2.7)_{1,3}$,

$$\mathbf{A}:\big(\mathbf{B}(\mathbf{e}\times)\big) = \mathbf{A}:\big(\mathbf{B}(\mathbf{e}\times)\mathbb{P}(\mathbf{e})\big) = \big(\mathbf{A}\mathbb{P}(\mathbf{e})\big):\big(\mathbf{B}(\mathbf{e}\times)\big).$$

For $\mathbf{A}$ a tensor, we write

$$\|\mathbf{A}\| = \sqrt{\mathbf{A}:\mathbf{A}} \tag{2.10}$$

for the *norm* of $\mathbf{A}$ and note that

$$\big\|\mathbf{A}\mathbb{P}(\mathbf{e})\big\|^2 = \big\|\mathbf{A}(\mathbf{e}\times)\big\|^2 = \big\|\mathbf{A}\big\|^2 - \big\|\mathbf{A}\mathbf{n}\big\|^2, \tag{2.11}$$

so that

$$\mathbf{A}\mathbb{P}(\mathbf{e}) = \mathbf{0} \quad \Leftrightarrow \quad \mathbf{A}(\mathbf{e}\times) = \mathbf{0}. \tag{2.12}$$

To verify (2.11), we write $\mathbb{P} = \mathbb{P}(\mathbf{e})$ and note that, by (2.7),

$$(\mathbf{A}\mathbb{P}):(\mathbf{A}\mathbb{P}) = -(\mathbf{A}\mathbb{P}):\big(\mathbf{A}(\mathbf{e}\times)(\mathbf{e}\times)\big) = \big(\mathbf{A}\mathbb{P}(\mathbf{e}\times)\big):\big(\mathbf{A}(\mathbf{e}\times)\big) = \big(\mathbf{A}(\mathbf{e}\times)\big):\big(\mathbf{A}(\mathbf{e}\times)\big),$$

which is the first equality in (2.11). Next, since $\mathbf{A}:(\mathbf{A}\mathbf{n}\otimes\mathbf{n}) = \|\mathbf{A}\mathbf{n}\|^2$ and $\|\mathbf{A}\mathbf{n}\otimes\mathbf{n}\|^2 = \|\mathbf{A}\mathbf{n}\|^2$, it follows that

$$\big\|\mathbf{A}\mathbb{P}\big\|^2 = \big\|\mathbf{A} - (\mathbf{A}\mathbf{n}\otimes\mathbf{n})\big\|^2 = \big\|\mathbf{A}(\mathbf{e}\times)\big\|^2 = \big\|\mathbf{A}\big\|^2 - \big\|\mathbf{A}\mathbf{n}\big\|^2,$$

which is the remainder of (2.11).

We close this section by establishing the following important result: given any tensor $\mathbf{A}$,

$$\underbrace{\mathbf{A}(\mathbf{m}\times):\mathbf{D} = 0 \quad \text{for every deviatoric tensor } \mathbf{D}}_{(\flat)} \qquad \Longrightarrow \qquad \mathbf{A}(\mathbf{m}\times) = \mathbf{0}. \tag{2.13}$$

Assume that $(\flat)$ is satisfied. Choose a tensor $\mathbf{S}$ and let $\mathbf{D} = \mathbf{S} - (\operatorname{tr}\mathbf{S})\mathbf{m}\otimes\mathbf{m}$. Then $\mathbf{D}$ is deviatoric and $\mathbf{A}(\mathbf{m}\times):\mathbf{S} = \mathbf{A}(\mathbf{m}\times):\mathbf{D}$, so that $\mathbf{A}(\mathbf{m}\times):\mathbf{S} = 0$. Since $\mathbf{S}$ was arbitrarily chosen, $\mathbf{A}(\mathbf{m}\times) = \mathbf{0}$.

2.3 Burgers-vector balance. Burgers-vector flow

Choose a *fixed* unit vector $\mathbf{e}$. Then the Burgers vector $\mathbf{G}^\top\mathbf{e}$ associated with small loops perpendicular to $\mathbf{e}$ evolves according to a balance. To derive this balance note that

$$e_i\epsilon_{ijk}\frac{\partial\dot{H}^p_{rk}}{\partial x_j} = \frac{\partial}{\partial x_j}\Big(\dot{H}^p_{rk}\epsilon_{kij}e_i\Big),$$

an identity whose left side represents $(\operatorname{curl}\dot{\mathbf{H}}^p)^\top\mathbf{e} = \overline{\dot{\mathbf{G}^\top\mathbf{e}}}$. We therefore have the *Burgers-vector balance*

$$\overline{\dot{\mathbf{G}^\top\mathbf{e}}} = -\operatorname{div}\big(-\dot{\mathbf{H}}^p(\mathbf{e}\times)\big) \tag{2.14}$$

in which $-\dot{\mathbf{H}}^p(\mathbf{e}\times)$ represents a *tensorial Burgers-vector flux*. An inspection of this balance shows that, given a plane $\Pi(\mathbf{n})$ with normal $\mathbf{n}$, $-\big(\dot{\mathbf{H}}^p(\mathbf{e}\times)\big)\mathbf{n}$ represents — for the Burgers vector associated with small loops perpendicular to $\mathbf{e}$ — the *Burgers-vector flow* across $\Pi(\mathbf{n})$ in the direction $\mathbf{n}$. Since

$$-\big(\dot{\mathbf{H}}^p(\mathbf{e}\times)\big)\mathbf{n} = -\dot{\mathbf{H}}^p(\mathbf{e}\times\mathbf{n}) = \dot{\mathbf{H}}^p(\mathbf{n}\times\mathbf{e}) = \big(\dot{\mathbf{H}}^p(\mathbf{n}\times)\big)\mathbf{e}, \tag{2.15}$$

flow in the direction $\mathbf{n}$ associated with small loops perpendicular to $\mathbf{e}$ is equal to the negative of the flow in the direction $\mathbf{e}$ associated with small loops perpendicular to $\mathbf{n}$. Therefore the tensor

$$\dot{\mathbf{H}}^p(\mathbf{n}\times) \tag{2.16}$$

represents the *Burgers-vector flow across* $\Pi(\mathbf{n})$; that is, $\dot{\mathbf{H}}^p(\mathbf{n}\times)$ applied to any unit vector $\mathbf{e}$ represents — for small loops perpendicular to $\mathbf{e}$ — the *flow of the Burgers-vector across* $\Pi(\mathbf{n})$ in the direction $\mathbf{n}$. Thus

$$\dot{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0} \tag{2.17}$$

at a particular point $\mathbf{x}$ on $\Pi(\mathbf{n})$ if and only if *there is no flow of the Burgers vector across* $\Pi(\mathbf{n})$ *at* $\mathbf{x}$.

2.4   Burgers vector for plane-strain with planar slip systems

Strict plane-strain

Under plane strain the displacement has the component form

$$u_i(x_1, x_2, t) \quad (i = 1, 2), \qquad u_3 = 0,$$

and results in a displacement gradient $\nabla\mathbf{u}$ that is independent of x_3, so that

$$(\nabla\mathbf{u})_{j3} = (\nabla\mathbf{u})_{3j} = 0 \quad (j = 1, 2, 3); \tag{2.18}$$

i.e.,

$$(\nabla\mathbf{u})\mathbf{e} = (\nabla\mathbf{u})^\top\mathbf{e} = \mathbf{0}, \qquad \text{with} \quad \mathbf{e} \equiv \mathbf{e}_3, \tag{2.19}$$

the *out-of-plane normal*.

When discussing plane deformations we restrict attention to *planar slip systems*; that is, slip systems α that satisfy

$$\mathbf{s}^\alpha \cdot \mathbf{e} = 0, \qquad \mathbf{m}^\alpha \cdot \mathbf{e} = 0, \qquad \mathbf{s}^\alpha \times \mathbf{m}^\alpha = \mathbf{e}, \tag{2.20}$$

with slips γ^α independent of x_3; all other slip systems are ignored. The assumption of planar slip systems yields restrictions on the components of $\mathbf{H}^p$ and (hence) $\mathbf{H}^e$, $\mathbf{E}^e$, and $\mathbf{W}^e$ strictly analogous to those of $\nabla\mathbf{u}$ as specified in (2.18) and (2.19). There is a large literature based on this *approximative* hypothesis. The resulting fully two-dimensional kinematics is important in constructing simple mathematical models, often based on two slip systems.[6]

Burgers vector g.   Burgers vector flow

The following notation for first and second *slip-directional derivatives* of a scalar field Φ and a vector field $\mathbf{v}$ is convenient:

$$\Phi_{,\beta} = \mathbf{s}^\beta \cdot \nabla\Phi, \qquad \Phi_{,\alpha\beta} = \mathbf{s}^\alpha \cdot (\nabla\nabla\Phi)\mathbf{s}^\beta, \qquad \mathbf{v}_{,\beta} = (\nabla\mathbf{v})\mathbf{s}^\beta. \tag{2.21}$$

Then, since $\mathbf{e} \cdot \nabla\gamma^\alpha = 0$, it follows that $\nabla\gamma^\alpha \times \mathbf{m}^\alpha = (\mathbf{s}^\alpha \cdot \nabla\gamma^\alpha)(\mathbf{s}^\alpha \times \mathbf{m}^\alpha) = \gamma^\alpha{}_{,\alpha}\,\mathbf{e}$, so that, by (2.3),

$$\mathbf{G} = \mathbf{e} \otimes \mathbf{g}, \qquad \mathbf{g} = \sum_\alpha \gamma^\alpha{}_{,\alpha}\,\mathbf{s}^\alpha. \tag{2.22}$$

Thus, since each slip direction $\mathbf{s}^\alpha$ is orthogonal to $\mathbf{e}$, it follows that $\mathbf{g} \perp \mathbf{e}$. Further, because $\mathbf{g} = \mathbf{G}^\top\mathbf{e}$, the vector $\mathbf{g}$ represents the *Burgers vector* (per unit area) for small loops on the cross-sectional plane (the plane with unit normal $\mathbf{e}$); for convenience, we restrict attention to such loops.

In discussing the flow of the Burgers vector we restrict attention to small loops perpendicular to $\mathbf{e}$. Then, by (1.4), (1.5), and (2.20)$_3$,

$$-\dot{\mathbf{H}}^p(\mathbf{e}\times) = \sum_\alpha \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes (\mathbf{e} \times \mathbf{m}^\alpha) = -\sum_\alpha \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \mathbf{s}^\alpha,$$

and the Burgers-vector balance (2.14) takes the simple form

$$\dot{\mathbf{g}} = -\mathrm{div}\left(\sum_\alpha \dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \mathbf{s}^\alpha\right) \qquad \left(\dot{g}_i = -\left(\sum_\alpha \frac{\partial\dot{\gamma}^\alpha}{\partial x_j} s_i^\alpha s_j^\alpha\right)\right). \tag{2.23}$$

In this case the *flow of the Burgers vector in the direction* $\mathbf{n}$ has the form

$$\sum_\alpha \dot{\gamma}^\alpha (\mathbf{s}^\alpha \cdot \mathbf{n})\mathbf{s}^\alpha. \tag{2.24}$$

---

[6]Cf., e.g., Asaro 1983, pp. 45-46, 84-97 and the references therein.

3 Principle of virtual power. Macroscopic and microscopic force balances

We write

$$\boldsymbol{\gamma} = (\gamma^1, \gamma^2, \ldots, \gamma^N)$$

for the list of slips. The theory presented here is based on the presumption that the power expended by each independent "rate-like" kinematical descriptor is expressible in terms of an associated force system consistent with its own balance. But the basic "rate-like" descriptors, namely $\dot{\mathbf{u}}$, $\dot{\mathbf{H}}^e$, and $\dot{\boldsymbol{\gamma}}$ are are not independent, as they are constrained by

$$\nabla \dot{\mathbf{u}} = \dot{\mathbf{H}}^e + \sum_\alpha \dot{\gamma}^\alpha \, \mathbb{S}^\alpha \tag{3.1}$$

(cf. (1.1), (1.2), (1.4)), and it is not apparent what forms the associated force balances should take. For that reason, we determine these balances using the principal of virtual power.

3.1 Principle of virtual power

Internal and external power expenditures

With each evolution of the body we associate macroscopic and microscopic force systems characterized by the manner in which they expend power. We assume that power is expended within the body in consort with elastic straining, with slip, and with the formation of defects; we therefore consider a system of stresses consisting of:

 (i) a *symmetric lattice stress* $\mathbf{T}$ that expends power over the lattice strain-rate $\dot{\mathbf{H}}^e$;

 (ii) a *defect stress* $\mathbb{T}$ that expends power over $\dot{\mathbf{G}}$ and hence over temporal changes in the Burgers vector;

 (iii) an *internal microforce* π^α for each slip system α; π^α expends power over the slip-rate $\dot{\gamma}^\alpha$.

Therefore, given any *part R* (subregion of the body), we assume that the power expended *within* R has the form

$$\mathcal{W}_{\text{int}}(R) = \int\limits_R (\mathbf{T} : \dot{\mathbf{H}}^e + \mathbb{T} : \operatorname{curl} \dot{\mathbf{H}}^p) \, dV + \sum_\alpha \int\limits_R \pi^\alpha \dot{\gamma}^\alpha \, dV \tag{3.2}$$

The internal power is balanced by power expended externally by tractions on ∂R and body forces acting within R. As is standard, we consider, as power conjugates for the macroscopic displacement $\mathbf{u}$, a *traction* $\mathbf{t}(\mathbf{n})$ (for each unit vector $\mathbf{n}$) and an external *body force* $\mathbf{f}$, presumed to *account for inertia*. The internal power (3.2) contains terms $\partial \dot{H}^p_{ij}/\partial x_k$ (because of the presence of $\operatorname{curl} \dot{\mathbf{H}}^p$) and — based on experience with other gradient theories — we assume that power is expended externally by a *defect traction* $\mathbf{X}(\mathbf{n})$ conjugate to the plastic-distortion rate $\dot{\mathbf{H}}^p$. We therefore assume that the *external* power expended on R has the form

$$\mathcal{W}_{\text{ext}}(R) = \int\limits_{\partial R} \mathbf{t}(\mathbf{n}) \cdot \dot{\mathbf{u}} \, dA + \int\limits_R \mathbf{f} \cdot \dot{\mathbf{u}} \, dV + \int\limits_{\partial R} \mathbf{X}(\mathbf{n}) : \dot{\mathbf{H}}^p \, dA. \tag{3.3}$$

We restrict attention to distortion rates $\dot{\mathbf{H}}^p$ that are consistent with (1.4) and hence that belong to the tensor space spanned by the Schmid tensors; consistent with this we require that $\mathbf{X}(\mathbf{n})$ also belong to this space:

$$\mathbf{X}(\mathbf{n}) \in \operatorname{span} \left\{ \mathbb{S}^\alpha : \ \alpha = 1, 2, \ldots N \right\} \tag{3.4}$$

Power expenditures in terms of slip-rates

We now show that, for each α, there are a *microstress* $\boldsymbol{\xi}^\alpha$ and a *microtraction* $\Xi^\alpha(\mathbf{n})$ such that

$$\left.\begin{aligned}
\mathbb{T}\!:\!\dot{\mathbf{G}} &= \sum_\alpha \boldsymbol{\xi}^\alpha \cdot \nabla\dot{\gamma}^\alpha, \\
\mathbf{X}(\mathbf{n})\!:\!\dot{\mathbf{H}}^p &= \sum_\alpha \Xi^\alpha(\mathbf{n})\dot{\gamma}^\alpha.
\end{aligned}\right\} \tag{3.5}$$

By (2.3) and the identity $\mathbf{A}\!:\!(\mathbf{a}\otimes\mathbf{b}) = A_{ij}a_i b_j$,

$$\mathbb{T}\!:\!\dot{\mathbf{G}} = \mathbb{T}\!:\!\sum_\alpha (\nabla\gamma^\alpha \times \mathbf{m}^\alpha)\otimes\mathbf{s}^\alpha = \sum_\alpha \mathbb{T}_{ij}\varepsilon_{irk}\frac{\partial\dot{\gamma}^\alpha}{\partial x_r}m_k^\alpha s_j^\alpha = \sum_\alpha \left(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha\right)\cdot\nabla\dot{\gamma}^\alpha$$

and this yields $(3.5)_1$ provided

$$\boldsymbol{\xi}^\alpha \stackrel{\text{def}}{=} \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha \equiv \mathbf{m}^\alpha \times (\mathbb{T}\mathbf{s}^\alpha) \qquad \left(\xi_i^\alpha = \varepsilon_{ijk}m_j^\alpha \mathbb{T}_{kr}s_r^\alpha\right) \tag{3.6}$$

for each α. On the other hand, by (1.5),

$$\mathbf{X}(\mathbf{n})\!:\!\dot{\mathbf{H}}^p = \sum_\alpha \gamma^\alpha \mathbf{X}(\mathbf{n})\!:\!\mathbb{S}^\alpha$$

and therefore, if we define

$$\Xi^\alpha(\mathbf{n}) \stackrel{\text{def}}{=} \mathbb{S}^\alpha\!:\!\mathbf{X}(\mathbf{n}) \qquad \left(\Xi^\alpha(\mathbf{n}) = \mathbb{S}_{ij}^\alpha X_{ij}(\mathbf{n})\right), \tag{3.7}$$

we are led to $(3.5)_2$.

Using (3.5), we may rewrite the internal and external power expenditures (3.2) and (3.3) in terms of slips and slip gradients (G-2002):

$$\left.\begin{aligned}
\mathcal{W}_{\text{int}}(R) &= \int_R \mathbf{T}\!:\!\dot{\mathbf{H}}^e \, dV + \sum_\alpha \int_R (\pi^\alpha\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla\dot{\gamma}^\alpha)\, dV, \\
\mathcal{W}_{\text{ext}}(R) &= \int_{\partial R} \mathbf{t}(\mathbf{n})\cdot\dot{\mathbf{u}}\, dA + \int_R \mathbf{f}\cdot\dot{\mathbf{u}}\, dV + \sum_\alpha \int_{\partial R} \Xi^\alpha(\mathbf{n})\dot{\gamma}^\alpha \, dA.
\end{aligned}\right\} \tag{3.8}$$

Virtual velocities. Principle of virtual power

Fix the time and consider the fields $\dot{\mathbf{u}}$, $\dot{\mathbf{H}}^e$, and $\dot{\boldsymbol{\gamma}}$ as virtual velocities to be specified independently in a manner consistent with (3.1); that is, denoting the virtual fields by $\tilde{\mathbf{u}}$, $\tilde{\mathbf{H}}^e$, and $\tilde{\boldsymbol{\gamma}}$ to distinguish them from fields associated with the actual evolution of the body, we require that

$$\nabla\tilde{\mathbf{u}} = \tilde{\mathbf{H}}^e + \sum_\alpha \tilde{\gamma}^\alpha \mathbb{S}^\alpha. \tag{3.9}$$

Further, we define a *generalized virtual velocity* to be a list

$$\mathcal{V} = (\tilde{\mathbf{u}}, \tilde{\mathbf{H}}^e, \tilde{\boldsymbol{\gamma}})$$

of such fields and write $\mathcal{W}_{\text{ext}}(R, \mathcal{V})$ and $\mathcal{W}_{\text{int}}(R, \mathcal{V})$ for $\mathcal{W}_{\text{ext}}(R)$ and $\mathcal{W}_{\text{int}}(R)$ when the actual fields $\dot{\mathbf{u}}$, $\dot{\mathbf{H}}^e$, and $\dot{\boldsymbol{\gamma}}$ are replaced by their virtual counterparts $\tilde{\mathbf{u}}$, $\tilde{\mathbf{H}}^e$, and $\tilde{\boldsymbol{\gamma}}$.

We postulate a *principle of virtual power* requiring that, given any generalized virtual velocity $\mathcal{V}$ and any part R,

(i) the corresponding internal and external virtual powers are balanced:

$$\mathcal{W}_{\text{ext}}(R, \mathcal{V}) = \mathcal{W}_{\text{int}}(R, \mathcal{V}); \tag{3.10}$$

(ii) the internal virtual power $\mathcal{W}_{\text{int}}(R, \mathcal{V})$ is invariant under superposed (infinitesimal) rigid rotations.

3.2 Macroscopic and microscopic force balances

In applying the power balance (3.10) we are at liberty to choose any $\mathcal{V}$ consistent with the constraint (3.9).

Macroscopic force and moment balance

Under a superposed rigid rotation, the only field associated with the the internal power that is not invariant is $\tilde{\mathbf{H}}^e$, which transforms to $\tilde{\mathbf{H}}^e + \mathbf{W}$, with $\mathbf{W}$ a skew tensor; thus a necessary and sufficient condition that the internal power be invariant is that

$$\int_R \mathbf{T} : \mathbf{W} \, dv = 0$$

for all skew tensors $\mathbf{W}$ and all all parts R; we therefore have the classical result

$$\mathbf{T} = \mathbf{T}^\top. \tag{3.11}$$

Consider next a generalized virtual velocity without slip ($\tilde{\boldsymbol{\gamma}} \equiv \mathbf{0}$); then $\nabla\tilde{\mathbf{u}} = \tilde{\mathbf{H}}^e$, $\mathbf{T} : \tilde{\mathbf{H}}^e = \mathbf{T} : \nabla\tilde{\mathbf{u}}$, and the power balance (3.10) takes the form

$$\int_{\partial R} \mathbf{t}(\mathbf{n}) \cdot \tilde{\mathbf{u}} \, dA = \int_R (\mathbf{T} : \nabla\tilde{\mathbf{u}} - \mathbf{f} \cdot \tilde{\mathbf{u}}) \, dV.$$

Equivalently,

$$\int_{\partial R} (\mathbf{t}(\mathbf{n}) - \mathbf{T}\mathbf{n}) \cdot \tilde{\mathbf{u}} \, dA = -\int_R \tilde{\mathbf{u}} \cdot (\operatorname{div} \mathbf{T} + \mathbf{f}) \, dV,$$

and since this relation must hold for all R and all $\tilde{\mathbf{u}}$, a standard argument leads to the traction condition

$$\mathbf{t}(\mathbf{n}) = \mathbf{T}\mathbf{n} \tag{3.12}$$

and the classical local force balance

$$\operatorname{div} \mathbf{T} + \mathbf{f} = \mathbf{0}. \tag{3.13}$$

Microscopic force balances

Consider a generalized virtual velocity with $\tilde{\mathbf{u}} \equiv \mathbf{0}$, choose the virtual field $\tilde{\boldsymbol{\gamma}}$ arbitrarily, so that, by (3.9),

$$\sum_\alpha \tilde{\gamma}^\alpha \left(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha\right) = -(\tilde{\mathbf{E}}^e + \tilde{\mathbf{W}}^e),$$

with $\tilde{\mathbf{E}}^e$ and $\tilde{\mathbf{W}}^e$ the symmetric and skew parts of $\tilde{\mathbf{H}}^e$. Then, since $\mathbf{T}$ is symmetric, $\mathbf{T} : \tilde{\mathbf{H}}^e = \mathbf{T} : \tilde{\mathbf{E}}^e = -\sum_\alpha \tau^\alpha \tilde{\gamma}^\alpha$, with

$$\tau^\alpha = \mathbf{s}^\alpha \cdot \mathbf{T}\mathbf{m}^\alpha = \mathbb{S}^\alpha : \mathbf{T} \tag{3.14}$$

the *resolved shear*, and the power balance (3.10) yields the *microscopic virtual-power relation*

$$\sum_\alpha \int_{\partial R} \Xi^\alpha(\mathbf{n})\tilde{\gamma}^\alpha \, dA = \sum_\alpha \int_R \left[(\pi^\alpha - \tau^\alpha)\tilde{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla\tilde{\gamma}^\alpha\right] dV \tag{3.15}$$

to be satisfied for all for all $\tilde{\boldsymbol{\gamma}}$ and all R. Equivalently,

$$\sum_\alpha \int_{\partial R} \left(\Xi^\alpha(\mathbf{n}) - \boldsymbol{\xi}^\alpha \cdot \mathbf{n}\right)\tilde{\gamma}^\alpha \, dA = -\sum_\alpha \int_R \left(\operatorname{div} \boldsymbol{\xi}^\alpha + \tau^\alpha - \pi^\alpha\right)\tilde{\gamma}^\alpha \, dV,$$

and arguing as before this yields the *microtraction conditions*

$$\Xi^\alpha(\mathbf{n}) = \boldsymbol{\xi}^\alpha \cdot \mathbf{n} \tag{3.16}$$

and the *microforce balances*

$$\operatorname{div} \boldsymbol{\xi}^\alpha + \tau^\alpha - \pi^\alpha = 0 \tag{3.17}$$

on each slip system α.

Microscopic balances and traction conditions in terms of $\mathbb{T}$

By (3.6),

$$\operatorname{div} \boldsymbol{\xi}^{\alpha} = m_k^{\alpha} \varepsilon_{rki} \frac{\partial \mathbb{T}_{ij}}{\partial x_r} s_j^{\alpha} = -m_k^{\alpha} \varepsilon_{kri} \frac{\partial \mathbb{T}_{ji}^{\top}}{\partial x_r} s_j^{\alpha} = -\mathbb{S}^{\alpha} \colon (\operatorname{curl} \mathbb{T}^{\top})^{\top},$$

and thus, since $\tau^{\alpha} = \mathbb{S}^{\alpha} \colon \mathbf{T}$, the microforce balances (3.17) may be written equivalently as

$$\mathbb{S}^{\alpha} \colon \left(-(\operatorname{curl} \mathbb{T}^{\top})^{\top} + \mathbf{T} \right) - \pi^{\alpha} = 0. \tag{3.18}$$

Further, by (3.6),

$$\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n} = m_k^{\alpha} \varepsilon_{rki} \mathbb{T}_{ij} s_j^{\alpha} n_r = -\varepsilon_{kri} n_r \mathbb{T}_{ij} m_k^{\alpha} s_j^{\alpha} = -\big((\mathbf{n}\times)\mathbb{T}\big) \colon \big(\mathbf{m}^{\alpha} \otimes \mathbf{s}^{\alpha}\big),$$

so that

$$\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n} = \mathbb{S}^{\alpha} \colon \big(\mathbb{T}^{\top}(\mathbf{n}\times)\big). \tag{3.19}$$

Thus $\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n}$ *is* $\mathbb{T}^{\top}(\mathbf{n}\times)$ *resolved on the α-th slip system*; hence *the N tractions $\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n}$ cannot generally be prescribed arbitrarily.* The result (3.19) has the immediate, but important, corollary:

$$\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n} = 0 \quad \text{for all } \alpha \qquad \Leftrightarrow \qquad \mathbb{S}^{\alpha} \colon \big(\mathbb{T}^{\top}(\mathbf{n}\times)\big) = \mathbf{0} \quad \text{for all } \alpha; \tag{3.20}$$

that is, $\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n} = 0$ for all α if and only if the orthogonal projection of $\mathbb{T}^{\top}(\mathbf{n}\times)$ onto the tensor subspace spanned by the Schmid tensors vanishes.

To determine the traction condition satisfied by $\mathbb{T}$, we note that, by (3.7), (3.16), and (3.19),

$$\mathbb{S}^{\alpha} \colon \big(\mathbf{X}(\mathbf{n}) - \mathbb{T}^{\top}(\mathbf{n}\times)\big) = 0 \qquad \text{for all } \alpha; \tag{3.21}$$

thus, since $\mathbf{X}(\mathbf{n})$ belongs to the space spanned by the Schmid tensors (cf. (3.4)), $\mathbf{X}(\mathbf{n})$ is the perpendicular projection of $\mathbb{T}^{\top}(\mathbf{n}\times)$ onto this space. Note that, by Cermelli's Theorem (footnote 3), for the special case of FCC or BCC crystals, (3.21) yields an explicit expression for the traction:

$$\mathbf{X}(\mathbf{n}) = \operatorname{dev}\big(\mathbb{T}^{\top}(\mathbf{n}\times)\big),$$

where $\operatorname{dev}(\dots)$ denotes the *deviatoric part* of $(\dots)$.

4   Energy imbalance

We consider a purely mechanical theory based on a second law in which *the temporal increase in free energy of any part R is less than or equal to the power expended on R.* Precisely, letting ψ denote the *free energy* per unit volume, we take the second law in the form of an energy imbalance asserting that

$$\overline{\int_R \psi \, dV} \leq \mathcal{W}_{\text{ext}}(R) \tag{4.1}$$

for all subbodies R. In view of (3.2), (3.3), the symmetry of $\mathbf{T}$, and the identity $\mathcal{W}_{\text{ext}}(R) = \mathcal{W}_{\text{int}}(R)$, (4.1) has the alternative forms

$$\left.\begin{aligned}
\overline{\int_R \psi \, dV} &\leq \int_{\partial R} \mathbf{T}\mathbf{n} \cdot \dot{\mathbf{u}} \, dA + \int_R \mathbf{f} \cdot \dot{\mathbf{u}} \, dV + \sum_{\alpha} \int_{\partial R} (\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n}) \dot{\gamma}^{\alpha} \, dA, \\
\overline{\int_R \psi \, dV} &\leq \int_R \mathbf{T} \colon \dot{\mathbf{E}}^e \, dV + \sum_{\alpha} \int_R (\pi^{\alpha} \dot{\gamma}^{\alpha} + \boldsymbol{\xi}^{\alpha} \cdot \nabla \dot{\gamma}^{\alpha}) \, dV.
\end{aligned}\right\} \tag{4.2}$$

Since R is arbitrary, $(4.2)_2$ yields the *free-energy inequality*

$$\dot{\psi} - \mathbf{T} \colon \dot{\mathbf{E}}^e - \sum_{\alpha} (\boldsymbol{\xi}^{\alpha} \cdot \nabla \dot{\gamma}^{\alpha} + \pi^{\alpha} \dot{\gamma}^{\alpha}) \leq 0, \tag{4.3}$$

or equivalently, by (3.5),

$$\dot{\psi} - \mathbf{T} \colon \dot{\mathbf{E}}^e - \mathbb{T} \colon \operatorname{curl} \dot{\mathbf{H}}^p + \pi^{\alpha} \dot{\gamma}^{\alpha} \leq 0. \tag{4.4}$$

We shall use this second inequality as a guide in developing a suitable constitutive theory.

5   Constitutive theory. Thermodynamic restrictions

Our goal is a theory that allows for constitutive dependences on $\mathbf{G}$, but that does not otherwise depart drastically from the classical theory. Toward this end, we begin with a constitutive equation for the free energy in which the classical elastic strain-energy is augmented by a *defect energy* $\Psi(\mathbf{G})$:

$$\psi = \tfrac{1}{2}\mathbf{E}^e \colon \mathbf{C}[\mathbf{E}^e] + \Psi(\mathbf{G}). \tag{5.1}$$

Let $\mathbf{G} = \mathbf{G}(t)$. Then, by (2.3),

$$\overline{\dot{\Psi(\mathbf{G})}} = \mathbb{T} \colon \dot{\mathbf{G}} = \sum_\alpha (\nabla \dot{\gamma}^\alpha \times \mathbf{m}^\alpha) \cdot \mathbb{T}\mathbf{s}^\alpha = \sum_\alpha \big(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha\big) \cdot \nabla \dot{\gamma}^\alpha, \tag{5.2}$$

showing that the normal slip-gradients $\mathbf{m}^\alpha \cdot \nabla \gamma^\alpha$ do not affect temporal changes in the defect energy. Next, by (5.1) and (5.2),

$$\dot{\psi} = \mathbf{C}[\mathbf{E}^e] \colon \dot{\mathbf{E}}^e + \sum_\alpha \big(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha\big) \cdot \nabla \dot{\gamma}^\alpha, \tag{5.3}$$

and the free-energy inequality (4.3) takes the form

$$\left\{\mathbf{T} - \mathbf{C}[\mathbf{E}^e]\right\} \colon \dot{\mathbf{E}}^e + \left\{\mathbb{T} - \frac{\partial \Psi(\mathbf{G})}{\partial \mathbf{G}}\right\} \colon \dot{\mathbf{G}} + \pi^\alpha \dot{\gamma}^\alpha \geq 0. \tag{5.4}$$

The left side of this inequality represents the *dissipation*, per unit volume. Consider constitutive equations giving $\mathbf{T}$, $\mathbb{T}$, and π^α as functions of $\mathbf{E}^e$, $\mathbf{G}$, and the list $\dot{\boldsymbol{\gamma}} = (\dot{\gamma}^1, \dot{\gamma}^2, \ldots, \dot{\gamma}^A)$ of slip-rates. We require that the inequality (5.4) hold for all choices of $\dot{\mathbf{E}}^e$, $\dot{\boldsymbol{\gamma}}$, and $\dot{\mathbf{G}}$; the linearity of this inequality in $\dot{\mathbf{E}}^e$ and $\dot{\mathbf{G}}$ then reduces the constitutive equation for $\mathbf{T}$ to the classical form

$$\mathbf{T} = \mathbf{C}[\mathbf{E}^e] \tag{5.5}$$

and — what is more important — requires that

$$\mathbb{T} = \frac{\partial \Psi(\mathbf{G})}{\partial \mathbf{G}}. \tag{5.6}$$

Thus (5.4) reduces to $\sum_\alpha \pi^\alpha \dot{\gamma}^\alpha \geq 0$. Guided by this inequality and more classical theories, we posit a constitutive relation for π^α in the form

$$\pi^\alpha = \sigma^\alpha f(\dot{\gamma}^\alpha), \tag{5.7}$$

where, for each fixed α,

$$f(\dot{\gamma}^\alpha) = -f(-\dot{\gamma}^\alpha), \qquad f(\dot{\gamma}^\alpha)\dot{\gamma}^\alpha \geq 0, \tag{5.8}$$

and where the *slip resistances* σ^α are consistent with the *hardening equations*

$$\dot{\sigma}^\alpha = \sum_\beta k^{\alpha\beta}(\sigma^1, \sigma^2, \ldots, \sigma^N, \mathbf{G})\,|\dot{\gamma}^\beta|, \qquad \sigma^\alpha(\mathbf{x}, 0) = 1, \tag{5.9}$$

The constitutive relations (5.1) and (5.5)–(5.9) are then consistent with the free-energy inequality. Note that π^α is dissipative, while $\boldsymbol{\xi}^\alpha$ is energetic. Note also that the constitutive theory is completely specified by the elasticity tensor $\mathbf{C}$, the defect energy Ψ, the *viscosity function* f, and the hardening moduli $k^{\alpha\beta}$; and that the dissipation is given by $\sum_\alpha \sigma^\alpha f(\dot{\gamma}^\alpha)\,\dot{\gamma}^\alpha$.

6   Viscoplastic flow rules

Given any slip system α, the microforce balance $\operatorname{div}\boldsymbol{\xi}^\alpha + \tau^\alpha - \pi^\alpha = 0$ — augmented by the relation $\boldsymbol{\xi}^\alpha = \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha$ and the constitutive equations for π^α and $\mathbb{T}$ — plays the role of a *viscoplastic flow rule* for α:

$$\tau^\alpha \; - \; \underbrace{(-1)\operatorname{div}\big(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha\big)}_{\substack{\text{backstress due to a} \\ \text{nonzero Burgers vector}}} \; = \; \underbrace{\sigma^\alpha f(\dot{\gamma}^\alpha)}_{\substack{\text{dissipative hard-} \\ \text{ening due to slip}}} \;, \qquad \mathbb{T} = \frac{\partial \Psi(\mathbf{G})}{\partial \mathbf{G}}. \tag{6.1}$$

Since $\mathbb{T} = \mathbb{T}(\mathbf{G})$, the *backstress* depends on $\mathbf{G}$ and $\nabla\mathbf{G}$, and hence on the first and second gradients $\nabla\gamma^\beta$ and $\nabla\nabla\gamma^\beta$, $\beta = 1, 2, \ldots, N$, thereby rendering the flow rule strongly *nonlocal*. Using the microforce balance in the form (3.18) we can write this flow rule alternatively as

$$\mathbb{S}^\alpha\colon \Big(-(\operatorname{curl}\mathbb{T}^\top)^\top + \mathbf{T} \Big) = \sigma^\alpha f(\dot{\gamma}^\alpha).$$

The flow rule (6.1) embodies two different hardening mechanisms: that provided by the hardening equations (5.9) and that which results, via the backstress, from an energetic dependence on $\mathbf{G}$.[7] Hardening imposed by by the hardening equation is *strictly dissipative*; hardening resulting from the backstress is *strictly energetic*.

7 Basic system of field equations

The *basic field equations* of the theory consist of:

- the *kinematical equations* (1.1), (1.2), (1.4), (2.2), and (2.3),

$$\left. \begin{aligned} \nabla\mathbf{u} = \mathbf{H}^e + \mathbf{H}^p, \qquad \mathbf{E}^e = \tfrac{1}{2}(\mathbf{H}^e + \mathbf{H}^{e\top}), \\ \mathbf{H}^p = \sum\nolimits_\alpha \gamma^\alpha \mathbb{S}^\alpha, \qquad \mathbf{G} = \operatorname{curl}\mathbf{H}^p = \sum\nolimits_\alpha (\nabla\gamma^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{s}^\alpha; \end{aligned} \right\} \tag{7.1}$$

- the *macroscopic balance* (3.13) supplemented by the stress-strain relation (5.5),

$$\operatorname{div}\mathbf{T} + \mathbf{f} = \mathbf{0}, \qquad \mathbf{T} = \mathbf{C}[\mathbf{E^e}], \tag{7.2}$$

- the *flow rule* (6.1), which is the microforce balance (3.17) supplemented by (3.6), the constitutive equations (5.6) and (5.7), and the hardening equations (5.9),

$$\left. \begin{aligned} \operatorname{div}\boldsymbol{\xi}^\alpha + \tau^\alpha = \pi^\alpha, \qquad \boldsymbol{\xi}^\alpha = \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha, \\ \mathbb{T} = \frac{\partial\Psi(\mathbf{G})}{\partial\mathbf{G}}, \qquad \pi^\alpha = \sigma^\alpha f(\dot{\gamma}^\alpha), \\ \dot{\sigma}^\alpha = \sum\nolimits_\beta k^{\alpha\beta}(\sigma^1, \sigma^2, \ldots, \sigma^N, \mathbf{G})\,|\dot{\gamma}^\beta|, \qquad \sigma^\alpha(\mathbf{x}, 0) = 1. \end{aligned} \right\} \tag{7.3}$$

8 Microscopically powerless boundary conditions

8.1 Microscopic power expenditure

The external power expended on a part R is given by (3.3) and the microscopic portion of this power is given by

$$\int_{\partial R} \underbrace{\mathbf{X}(\mathbf{n})\colon\dot{\mathbf{H}}^p}_{M(\mathbf{n})}\, dA. \tag{8.1}$$

The integrand $M(\mathbf{n})$ represents the microscopic power expended, per unit area, on any (oriented) surface with unit normal $\mathbf{n}$. Multiplying (3.21) by $\dot{\gamma}^\alpha$ and summing over α, we find, using (1.4), that

$$M(\mathbf{n}) \overset{\text{def}}{=} \mathbf{X}(\mathbf{n})\colon\dot{\mathbf{H}}^p = \big(\mathbb{T}^\top(\mathbf{n}\times)\big)\colon\dot{\mathbf{H}}^p \qquad \big(M(\mathbf{n}) = \mathbb{S}^\alpha_{ij}X_{ij}(\mathbf{n}) = \mathbb{T}_{ji}\varepsilon_{jkl}n_k\dot{H}^p_{il}\big), \tag{8.2}$$

which is the first of the following expressions for this power:

$$M(\mathbf{n}) = \big(\mathbb{T}^\top(\mathbf{n}\times)\big)\colon\dot{\mathbf{H}}^p, \tag{8.3}$$

$$= -\mathbb{T}^\top\mathbb{P}(\mathbf{n})\colon\big(\dot{\mathbf{H}}^p(\mathbf{n}\times)\big), \tag{8.4}$$

$$= \sum_\alpha (\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot{\gamma}^\alpha. \tag{8.5}$$

The identity (8.4) follows from (2.8), while (8.5) follows from (3.16), (3.19), and (8.3).

---

[7]Cf. the discrete-dislocation computations of Cleveringa, Van der Giessen, and Needleman (1999), which display large backstresses.

8.2 Microhard and microfree boundary conditions

Focusing on the boundary ∂B, with outward unit normal $\mathbf{n}$, the quantity $M(\mathbf{n})$ defined in (8.2) represents the microscopic power expended, per unit area, on ∂B by the material in contact with the body. We here limit our discussion to boundary conditions that are *microscopically powerless* in the sense that

$$M(\mathbf{n}) = 0 \quad \text{on} \ \ \partial B. \tag{8.6}$$

Let $\mathcal{S}_{\text{hard}}$ and $\mathcal{S}_{\text{free}}$ denote complementary subsurfaces of ∂B. We consider the boundary condition

$$\dot{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0} \quad \text{on} \ \ \mathcal{S}_{\text{hard}} \qquad (\textbf{microhard condition}) \tag{8.7}$$

asserting that *there be no flow of the Burgers-vector across* $\mathcal{S}_{\text{hard}}$ (cf. §2.3, §8.3). We supplement (8.7) by the requirement that $\mathbf{X}(\mathbf{n}) = \mathbf{0}$ on $\mathcal{S}_{\text{free}}$, or, equivalently, by (3.4), (3.19), and (3.21), that either of the following two *equivalent* boundary conditions are satisfied:

$$\left. \begin{array}{r} \mathbb{S}^\alpha\colon \left(\mathbb{T}^\top(\mathbf{n}\times)\right) = 0 \quad \text{on} \ \ \mathcal{S}_{\text{free}} \quad \text{for all } \alpha \\[4pt] \boldsymbol{\xi}^\alpha \cdot \mathbf{n} = 0 \quad \text{on} \ \ \mathcal{S}_{\text{free}} \quad \text{for all } \alpha \end{array} \right\} \quad (\textbf{microfree condition}), \tag{8.8}$$

When expressed in indicial notation, the microhard condition and the (first) microfree condition have the form

$$\dot{H}^p_{ij}\varepsilon_{jkl}n_k = 0 \quad \text{on} \ \ \mathcal{S}_{\text{hard}} \qquad \text{and} \qquad \mathbb{S}^\alpha_{ij}\mathbb{T}_{ri}\varepsilon_{rkj}n_k = 0 \quad \text{on} \ \ \mathcal{S}_{\text{free}}..$$

Note that, for FCC and BCC crystals we may use the discussion of footnote 3 to rewrite the microfree condition in the form

$$\text{dev}\left(\mathbb{T}^\top(\mathbf{n}\times)\right) = 0 \quad \text{on} \ \ \mathcal{S}_{\text{free}}. \tag{8.9}$$

The following remark is a direct consequence of (8.3) and (8.5):

(#) *The microhard and microfree boundary conditions together imply that $M(\mathbf{n}) = 0$ on ∂B.*

8.3 Microhard boundary points

General results

A boundary point is *microhard* if, there, $\dot{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0}$, or, equivalently, by (2.12), if

$$\dot{\mathbf{H}}^p\mathbb{P}(\mathbf{n}) = \mathbf{0}. \tag{8.10}$$

An interesting and important property of a microhard boundary point is that, at that point, $\dot{\mathbf{H}}^p$ represents *single slip with slip-plane tangent to the boundary*:

$$\dot{\mathbf{H}}^p = \mathbf{b} \otimes \mathbf{n}, \qquad \mathbf{b} \perp \mathbf{n}. \tag{8.11}$$

To verify (8.11) note first that, by (8.10),

$$\dot{\mathbf{H}}^p\mathbb{P}(\mathbf{n}) = \dot{\mathbf{H}}^p(\mathbf{1} - \mathbf{n}\otimes\mathbf{n}) = \dot{\mathbf{H}}^p - (\dot{\mathbf{H}}^p\mathbf{n})\otimes\mathbf{n}.$$

Thus, defining $\mathbf{b} = \dot{\mathbf{H}}^p\mathbf{n}$, it follows that $\dot{\mathbf{H}}^p\mathbb{P}(\mathbf{n}) = \mathbf{0}$ if and only if $\dot{\mathbf{H}}^p = \mathbf{b}\otimes\mathbf{n}$ (with $\mathbf{b} \perp \mathbf{n}$ since $\text{tr}\,\dot{\mathbf{H}}^p = 0$).

We next show that *if the entire boundary is microhard, then the mean value of the Burgers tensor is constant*:

$$\frac{d}{dt}\int_B \mathbf{G}\,dV = \mathbf{0}. \tag{8.12}$$

By hypothesis, $\dot{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0}$ on ∂B. Choose an arbitrary unit vector $\mathbf{e}$. Then (2.14), the divergence theorem, and (2.15) imply that,

$$\frac{d}{dt}\int_B \mathbf{G}^\top\mathbf{e}\,dV = \int_{\partial B} \dot{\mathbf{H}}^p(\mathbf{e}\times\mathbf{n})\,dA = -\int_{\partial B} \dot{\mathbf{H}}^p(\mathbf{n}\times\mathbf{e})\,dA = \mathbf{0}.$$

Since $\mathbf{e}$ is constant and arbitrary, this yields $(d/dt)\int_B \mathbf{G}^\top dV = \mathbf{0}$; the transpose of this relation is (8.12).

The microhard condition for single- and double-slip

In the case of *single-slip* the microhard condition $\dot{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0}$ takes the form

$$\dot{\gamma}\mathbf{s} \otimes (\mathbf{m} \times \mathbf{n}) = 0 \tag{8.13}$$

and requires that *either the slip plane is parallel to the boundary or $\dot{\gamma} = 0$*.

   Consider next *double-slip* and let $\{\beta, \kappa\}$ label the slip systems, so that

$$\dot{\mathbf{H}}^p = \dot{\gamma}^\beta \mathbf{s}^\beta \otimes \mathbf{m}^\beta + \dot{\gamma}^\kappa \mathbf{s}^\kappa \otimes \mathbf{m}^\kappa.$$

The microhard condition is then equivalent to the requirement that

$$\dot{\gamma}^\beta \mathbf{s}^\beta \otimes (\mathbf{n} \times \mathbf{m}^\beta) + \dot{\gamma}^\kappa \mathbf{s}^\kappa \otimes (\mathbf{n} \times \mathbf{m}^\kappa) = \mathbf{0}. \tag{8.14}$$

As a consequences of (8.14),

   (i) if both slip planes are parallel to the boundary, then the microhard condition is satisfied automatically;

   (ii) if just one slip plane, say κ, is parallel to the boundary, then the microhard condition requires that $\dot{\gamma}^\beta = 0$;

   (iii) if neither slip plane is parallel to the boundary, then either

   (a) $\mathbf{s}^\beta \neq \mathbf{s}^\kappa$ and $\dot{\gamma}^\beta = \dot{\gamma}^\kappa = 0$, or

   (b) $\mathbf{s}^\beta = \mathbf{s}^\kappa$ and $\dot{\gamma}^\beta \mathbf{m}^\beta + \dot{\gamma}^\kappa \mathbf{m}^\kappa$ is parallel to $\mathbf{n}$.

Conversely, each of the conditions (i)-(iii) implies (8.14).

Plane strain with planar slip systems

In this case $\dot{\mathbf{H}}^p \mathbf{e} = \mathbf{0}$ and, for any vector $\mathbf{t}$ orthogonal to $\mathbf{e}$, $\dot{\mathbf{H}}^p(\mathbf{n} \times \mathbf{t}) = \mathbf{0}$. Thus $\dot{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0}$ is equivalent to $\dot{\mathbf{H}}^p(\mathbf{n}\times)\mathbf{e} = \mathbf{0}$ and hence, by (2.20), to

$$\mathbf{0} = \dot{\mathbf{H}}^p(\mathbf{e}\times)\mathbf{n} = \sum_\alpha \left(\dot{\gamma}^\alpha \mathbf{s}^\alpha \otimes \underbrace{(\mathbf{m}^\alpha \times \mathbf{e})}_{\mathbf{s}^\alpha} \right) \mathbf{n}.$$

Thus the microhard boundary condition is equivalent to the requirement that

$$\sum_\alpha \dot{\gamma}^\alpha (\mathbf{s}^\alpha \cdot \mathbf{n}) \mathbf{s}^\alpha = \mathbf{0}. \tag{8.15}$$

9   Uniqueness theorem

We now establish uniqueness for the boundary-value problem associated with:

(P1) the *field equations* (7.1)-(7.3) for a prescribed body force $\mathbf{f}$;

(P2) *constitutive assumptions* requiring that:

   (i) the elasticity tensor $\mathbf{C}$ be symmetric and the elastic energy positive-definite,

$$w(\mathbf{E}^e) \overset{\text{def}}{=} \tfrac{1}{2}\mathbf{E}^e : \mathbf{C}[\mathbf{E}^e] > 0 \ \text{ for } \ \mathbf{E}^e \neq 0; \tag{9.1}$$

   (ii) the defect energy $\Psi(\mathbf{G})$ be quadratic and positive-definite;

   (iii) the hardening moduli $k^{\alpha\beta}$ vanish, so that, for all α, $\sigma^\alpha = 1$ and

$$\pi^\alpha = f(\dot{\gamma}^\alpha); \tag{9.2}$$

(iv) f be strictly increasing;

(P3) the (standard) macroscopic *boundary conditions*

$$\mathbf{u} = \hat{\mathbf{u}} \quad \text{on} \ \ \mathcal{S}_{\text{dis}} \quad \text{and} \quad \mathbf{Tn} = \hat{\mathbf{t}} \quad \text{on} \ \ \mathcal{S}_{\text{trac}}, \tag{9.3}$$

with $\mathcal{S}_{\text{dis}}$ and $\mathcal{S}_{\text{trac}}$ complementary subsets of ∂B and $\hat{\mathbf{u}}$ and $\hat{\mathbf{t}}$ prescribed functions;

(P4) the *microhard and microfree boundary conditions* (8.7) and (8.9);

(P5) *initial conditions* prescribing $\mathbf{u}$ and $\gamma^1, \gamma^2, \ldots, \gamma^N$ at $t = 0$.

We consider two solutions of this boundary-value problem and denote the underlying fields by $\mathbf{u}_1$, γ_1^α, $\mathbf{T}_1$, $\boldsymbol{\xi}_1^\alpha$, etc. and $\mathbf{u}_2$, γ_2^α, $\mathbf{T}_2$, $\boldsymbol{\xi}_2^\alpha$, etc. Further, we denote the corresponding difference fields by $\mathbf{u} = \mathbf{u}_1 - \mathbf{u}_2$, $\gamma^\alpha = \gamma_1^\alpha - \gamma_2^\alpha$, $\mathbf{T} = \mathbf{T}_1 - \mathbf{T}_2$, $\boldsymbol{\xi}^\alpha = \boldsymbol{\xi}_2^\alpha - \boldsymbol{\xi}_1^\alpha$, and so forth. Then, by (P1) and (P2),

$$\operatorname{div} \mathbf{T} = \mathbf{0}, \qquad \operatorname{div} \boldsymbol{\xi}^\alpha + \tau^\alpha = f(\dot{\gamma}_1^\alpha) - f(\dot{\gamma}_2^\alpha) \ \ (\text{for all } \alpha). \tag{9.4}$$

By $(9.4)_1$ and the divergence theorem,

$$\int_{\partial B} \mathbf{Tn} \cdot \dot{\mathbf{u}} \, dA = \int_B \mathbf{T} : \nabla \dot{\mathbf{u}} \, dV.$$

The boundary conditions for the difference fields $\mathbf{u}$ and $\mathbf{T}$ are (9.3) with $\hat{\mathbf{u}} = \mathbf{0}$ and $\hat{\mathbf{t}} = \mathbf{0}$, so that $\mathbf{Tn} \cdot \dot{\mathbf{u}} = 0$; thus, since $\nabla \dot{\mathbf{u}} = \dot{\mathbf{H}}^e + \dot{\mathbf{H}}^p$ and $\mathbf{T}$ is symmetric,

$$\int_B \mathbf{T} : \dot{\mathbf{E}}^e \, dV = - \int_B \mathbf{T} : \dot{\mathbf{H}}^p \, dV. \tag{9.5}$$

Next, multiplying $(9.4)_2$ by $\dot{\gamma}^\alpha$, summing over α, and integrating over B, we find that

$$\sum_\alpha \int_B \left(\dot{\gamma}^\alpha \operatorname{div} \boldsymbol{\xi}^\alpha + \tau^\alpha \dot{\gamma}^\alpha \right) dV = \sum_\alpha \int_B \left(f(\dot{\gamma}_1^\alpha) - f(\dot{\gamma}_2^\alpha) \right) \left(\dot{\gamma}_1^\alpha - \dot{\gamma}_2^\alpha \right) dV. \tag{9.6}$$

On the other hand, by (1.4), $(3.5)_1$, (3.14), and (3.19),

$$\sum_\alpha \boldsymbol{\xi}^\alpha \cdot \nabla \dot{\gamma}^\alpha = \mathbb{T} : \dot{\mathbf{G}}, \qquad \sum_\alpha \tau^\alpha \dot{\gamma}^\alpha = \mathbf{T} : \dot{\mathbf{H}}^p, \qquad \sum_\alpha (\boldsymbol{\xi}^\alpha \cdot \mathbf{n}) \dot{\gamma}^\alpha = \mathbb{T}^\top (\mathbf{n} \times) : \dot{\mathbf{H}}^p,$$

and therefore

$$\sum_\alpha \int_B \left(\dot{\gamma}^\alpha \operatorname{div} \boldsymbol{\xi}^\alpha + \tau^\alpha \dot{\gamma}^\alpha \right) dV = \sum_\alpha \int_{\partial B} (\boldsymbol{\xi}^\alpha \cdot \mathbf{n}) \dot{\gamma}^\alpha \, dA + \sum_\alpha \int_B \left(\tau^\alpha \dot{\gamma}^\alpha - \boldsymbol{\xi}^\alpha \cdot \nabla \dot{\gamma}^\alpha \right) dV$$

$$= \int_{\partial B} \mathbb{T}^\top (\mathbf{n} \times) : \dot{\mathbf{H}}^p \, dA + \int_B \left(\mathbf{T} : \dot{\mathbf{H}}^p - \mathbb{T} : \dot{\mathbf{G}} \right) dV. \tag{9.7}$$

The results (9.6) and (9.7) imply that

$$\int_{\partial B} \left(\mathbb{T}^\top (\mathbf{n} \times) : \dot{\mathbf{H}}^p \right) dA + \int_B \left(- \mathbb{T} : \dot{\mathbf{G}} + \mathbf{T} : \dot{\mathbf{H}}^p \right) dV = \sum_\alpha \int_B \left(f(\dot{\gamma}_1^\alpha) - f(\dot{\gamma}_2^\alpha) \right) \left(\dot{\gamma}_1^\alpha - \dot{\gamma}_2^\alpha \right) dV. \tag{9.8}$$

By (P4), the remark ($\flat$) on page 14, and (8.2), the integral in (9.8) over ∂B vanishes, so that, by (9.5),

$$- \int_B \left(\mathbb{T} : \dot{\mathbf{G}} + \mathbf{T} : \dot{\mathbf{E}}^e \right) dV = \sum_\alpha \int_B \left(f(\dot{\gamma}_1^\alpha) - f(\dot{\gamma}_2^\alpha) \right) \left(\dot{\gamma}_1^\alpha - \dot{\gamma}_2^\alpha \right) dV. \tag{9.9}$$

Moreover, because the elastic energy $w(\mathbf{E}^e)$ and the defect energy $\Psi(\mathbf{G})$ are quadradic, the difference fields satisfy

$$\mathbb{T}:\dot{\mathbf{G}} + \mathbf{T}:\dot{\mathbf{E}}^e = \overline{\dot{w(\mathbf{E}^e) + \Psi(\mathbf{G})}}.$$

We therefore have the following basic identity for the difference fields

$$-\overline{\int_B \dot{\left(w(\mathbf{E}^e) + \Psi(\mathbf{G})\right)} \, dV} = \int_B \left(f(\dot{\gamma}_1^\alpha) - f(\dot{\gamma}_2^\alpha)\right)\left(\dot{\gamma}_1^\alpha - \dot{\gamma}_2^\alpha\right) dV. \tag{9.10}$$

By hypothesis, f is strictly increasing; thus the right side of (9.10) is ≥ 0 and the total difference energy $\int_B \left(w(\mathbf{E}^e) + \Psi(\mathbf{G})\right) dV$ must decrease in time. But the initial conditions (P5) imply that $\mathbf{E}^e$ and $\mathbf{G}$ vanish initially. Thus since, by (P2), the elastic and defect energies are positive definite, $\mathbf{E}^e$ and $\mathbf{G}$ must vanish identically. Therefore

$$\int_B \left(f(\dot{\gamma}_1^\alpha) - f(\dot{\gamma}_2^\alpha)\right)\left(\dot{\gamma}_1^\alpha - \dot{\gamma}_2^\alpha\right) dV = 0, \tag{9.11}$$

which — because f is strictly increasing — is possible only if the slip-rate differences $\dot{\gamma}^\alpha = \dot{\gamma}_1^\alpha - \dot{\gamma}_2^\alpha$ vanish identically. Since these differences vanish initially, they must vanish identically, as must $\mathbf{H}^p$. Thus, as $\mathbf{E}^e = \mathbf{0}$, $\nabla\mathbf{u}$ is skew and the displacements of the two solutions differ by a rigid displacement. We therefore have the

Uniqueness Theorem The boundary-value problem defined by (P1)-(P4) has at most one solution up to a rigid displacement of the entire body.[8]

10 Variational formulation of the microforce balance and microfree boundary conditions

Our goal is a variational formulation of the *microforce balance* (3.17) — and hence the flow rule, granted constitutive equations — that encapsulates the microfree boundary condition (8.9). We work within the framework of the microhard and microfree boundary conditions and therefore begin with the microscopic virtual-power relation (3.15) applied to $R = B$. Because the boundary conditions render the power expenditure $M(\mathbf{n})$ null on ∂B, we consider (3.15) with the boundary term omitted:

$$\sum_\alpha \int_B \left((\pi^\alpha - \tau^\alpha)\tilde{\gamma}^\alpha + \boldsymbol{\xi}^\alpha \cdot \nabla\tilde{\gamma}^\alpha\right) dV = 0. \tag{10.1}$$

In view of the microhard boundary condition (8.7), we restrict attention to *kinematically admissible* slip-rates; that is, slip-rates $\tilde{\boldsymbol{\gamma}} = (\tilde{\gamma}^1, \tilde{\gamma}^2, \ldots, \tilde{\gamma}^N)$ that satisfy

$$\tilde{\mathbf{H}}^p(\mathbf{n}\times) = \mathbf{0} \quad \text{on} \quad \mathcal{S}_{\text{hard}}, \tag{10.2}$$

where

$$\tilde{\mathbf{H}}^p \stackrel{\text{def}}{=} \sum_\alpha \tilde{\gamma}^\alpha \mathbb{S}^\alpha. \tag{10.3}$$

Integrating the term $\boldsymbol{\xi}^\alpha \cdot \nabla\tilde{\gamma}^\alpha$ in (10.1) by parts, we are led to the relation

$$\sum_\alpha \int_{\partial B} (\boldsymbol{\xi}^\alpha \cdot \mathbf{n})\tilde{\gamma}^\alpha \, dA = \sum_\alpha \int_B \left(\text{div}\,\boldsymbol{\xi}^\alpha + \tau^\alpha - \pi^\alpha\right)\tilde{\gamma}^\alpha \, dV.$$

---

[8]The extension of this result to include the hardening equations (5.9) is technical and beyond the scope of the present study.

By (8.3)-(8.5) (which hold with the rate terms replaced by variations)

$$\sum_\alpha \int_{\partial B} (\boldsymbol{\xi}^\alpha \cdot \mathbf{n}) \tilde{\gamma}^\alpha \, dA \; = \sum_\alpha \int_{\mathcal{S}_{\text{free}}} \left(\mathbb{T}^\top (\mathbf{n} \times) \right) : \dot{\mathbf{H}}^p \, dA \; - \underbrace{\int_{\mathcal{S}_{\text{hard}}} \mathbb{T}^\top : \left(\tilde{\mathbf{H}}^p (\mathbf{n} \times) \right) dA}_{= \mathbf{0} \text{ by (10.2)}},$$

Thus, by (10.3),

$$\sum_\alpha \int_{\mathcal{S}_{\text{free}}} \tilde{\gamma}^\alpha \, \mathbb{S}^\alpha : \left(\mathbb{T}^\top (\mathbf{n} \times) \right) dA = \sum_\alpha \int_B \left(\operatorname{div} \boldsymbol{\xi}^\alpha + \tau^\alpha - \pi^\alpha \right) \tilde{\gamma}^\alpha \, dV \tag{10.4}$$

for all kinematically admissible slip-rates $\tilde{\boldsymbol{\gamma}}$. Thus, restricting attention, for the moment, to $\tilde{\boldsymbol{\gamma}}$ that vanish on the boundary, the fundamental lemma of the calculus of variations yields the microforce balance (3.17) and reduces (10.4) to

$$\sum_\alpha \int_{\mathcal{S}_{\text{free}}} \tilde{\gamma}^\alpha \, \mathbb{S}^\alpha : \left(\mathbb{T}^\top (\mathbf{n} \times) \right) dA = 0. \tag{10.5}$$

Since the virtual fields $\tilde{\gamma}^\alpha$ are unconstrained on $\mathcal{S}_{\text{free}}$, the microfree conditions $\mathbb{S}^\alpha : \left(\mathbb{T}^\top (\mathbf{n} \times) \right) = 0$ (for all α) must be satisfied on $\mathcal{S}_{\text{free}}$. We have therefore established the

> **Variational Formulation**. Assume that (10.1) is satisfied for all kinematically admissible slip-rates $\tilde{\boldsymbol{\gamma}}$. Then the microforce balance (3.17) is satisfied, as is the microfree boundary condition (8.9).

11 Grain boundaries

11.1 Kinematics

Consider a *grain boundary* $\mathcal{G}$ separating grains G_1 and G_2, and let $\mathbf{n}$ denote the unit normal field on $\mathcal{G}$ directed outward from grain 1. We assume that the fields under consideration are smooth in each grain and continuous up to $\mathcal{G}$ from either grain. Given such a field Φ, we write Φ_1 and Φ_2 for the (one-sided) limits of Φ at $\mathcal{G}$ from G_1 and G_2, $[\![\Phi]\!]$ for the *jump* in Φ across $\mathcal{G}$, and $\langle\!\langle \Phi \rangle\!\rangle$ for the *average value* of Φ at $\mathcal{G}$:

$$[\![\Phi]\!] = \Phi_2 - \Phi_1, \qquad \langle\!\langle \Phi \rangle\!\rangle = \tfrac{1}{2}(\Phi_2 + \Phi_1).$$

We then have the identity

$$[\![\Phi\Lambda]\!] = \langle\!\langle \Phi \rangle\!\rangle [\![\Lambda]\!] + \langle\!\langle \Lambda \rangle\!\rangle [\![\Phi]\!]. \tag{11.1}$$

We let $\mathbf{Q}$ denote the orthogonal tensor that represents the *misorientation* of the grains, so that, for $\mathbb{S}_1^\alpha$ and $\mathbb{S}_2^\alpha$ the Schmid tensors of G_1 and G_2,

$$\mathbb{S}_2^\alpha = \mathbf{Q}\mathbb{S}_1^\alpha \mathbf{Q}^\top; \tag{11.2}$$

i.e.,

$$\mathbf{s}_2^\alpha = \mathbf{Q}\mathbf{s}_1^\alpha, \qquad \mathbf{m}_2^\alpha = \mathbf{Q}\mathbf{m}_1^\alpha. \tag{11.3}$$

We assume that the displacement $\mathbf{u}$ is continuous across $\mathcal{G}$,

$$[\![\mathbf{u}]\!] = \mathbf{0}; \tag{11.4}$$

we therefore do not account for the relative slip between grains.

Burgers-vector flows at the grain-boundary. Permeability to Burgers-vector flows

Choose an arbitrary point $\mathbf{x}$ on the grain boundary and an arbitrary line element $\mathbf{dx}$ at that point *tangent* to $\mathcal{G}$. Consider the "infinitesimal loop" $d\Gamma$ consisting of $\mathbf{dx}$ in Grain 1 followed by $-\mathbf{dx}$ in Grain 2, and note that $-\mathbf{n} \times \mathbf{dx}$ represents a unit normal to the "surface element" bounded by $d\Gamma$. (The minus sign renders the normal $-\mathbf{n} \times \mathbf{dx}$ "righthanded" with respect to the orientation of $d\Gamma$ and hence consistent with the convention tacit in §5. Then the *Burgers vector* corresponding to the "loop" $d\Gamma$ is given by

$$\mathbf{H}_1^p \mathbf{dx} - \mathbf{H}_2^p \mathbf{dx} = (\mathbf{H}_1^p - \mathbf{H}_2^p)\mathbf{dx} = -[\![\mathbf{H}^p]\!]\mathbf{dx} = -[\![\mathbf{H}^p]\!]\,\mathbb{P}(\mathbf{n})\mathbf{dx} = \big([\![\mathbf{H}^p]\!](\mathbf{n}\times)\big)(\mathbf{n}\times\mathbf{dx}), \qquad (11.5)$$

where the insertion of the projection $\mathbb{P}(\mathbf{n})$ is valid because $\mathbf{dx}$ is tangent to $\mathcal{G}$, and where we have used the identity (2.7) in the last step in (11.5). Since the point $\mathbf{x}$ and the line element $\mathbf{dx}$ at $\mathbf{x}$ tangent to $\mathcal{G}$ were arbitrarily chosen, (11.5) allows us to identify

$$-[\![\mathbf{H}^p]\!](\mathbf{n}\times)$$

as the *Burgers-vector density of the grain boundary*, measured per unit length. We refer to the grain boundary as *defect-free* if $[\![\mathbf{H}^p]\!](\mathbf{n}\times) = \mathbf{0}$.

Next, in view of the discussion in the sentence containing (2.16),

$$-[\![\dot{\mathbf{H}}^p]\!](\mathbf{n}\times) = \dot{\mathbf{H}}_2^p((-\mathbf{n})\times) + \dot{\mathbf{H}}_1^p\big(\mathbf{n}\times\big) \qquad (11.6)$$

gives the Burgers-vector flow into $\mathcal{G}$ from the grains and hence represents the Burgers-vector production within the grain boundary. Thus, trivially, the Burgers-vector flow into $\mathcal{G}$ is balanced by the rate at which the Burgers-vector density of $\mathcal{G}$ is increasing. Further, the condition

$$[\![\dot{\mathbf{H}}^p]\!](\mathbf{n}\times) = \mathbf{0} \qquad \big([\![\dot{H}_{ij}^p]\!]\varepsilon_{jrl}n_r = 0\big) \qquad (11.7)$$

represents a balanced Burgers-vector flow in which *the flow out of, say, Grain 1 is equal to the flow into Grain 2*. When (11.7) is satisfied we say that $\mathcal{G}$ is *permeable to Burgers-vector flow*; we note that if $\mathcal{G}$ is permeable, then $\mathcal{G}$ is defect-free if it ever once was.

Finally, the fact that permeable grain boundaries allow for the unimpeded flow of the Burgers vector leads us to make the following:

> $(*)$ **Conjecture**. For a given problem involving a grain boundary $\mathcal{G}$ — and away from any influence of the outer boundaries — solutions within our theory for $\mathcal{G}$ permeable would be qualitatively similar to solutions within more clsssical theories that do not account constitutively for the Burgers vector.

Transition conditions for double-slip at a permeable grain-boundary

Let $\{\varphi, \kappa\}$ and $\{\bar{\varphi}, \bar{\kappa}\}$ label the slip systems, so that $[\![\dot{\mathbf{H}}^p]\!](\mathbf{n}\times) = \mathbf{0}$ becomes

$$\dot{\gamma}^\varphi \mathbf{s}^\varphi \otimes (\mathbf{n}\times\mathbf{m}^\varphi) + \dot{\gamma}^\kappa \mathbf{s}^\kappa \otimes (\mathbf{n}\times\mathbf{m}^\kappa) = \dot{\gamma}^{\bar{\varphi}} \mathbf{s}^{\bar{\varphi}} \otimes (\mathbf{n}\times\mathbf{m}^{\bar{\varphi}}) + \dot{\gamma}^{\bar{\kappa}} \mathbf{s}^{\bar{\kappa}} \otimes (\mathbf{n}\times\mathbf{m}^{\bar{\kappa}}); \qquad (11.8)$$

here $\big(\mathbf{a}\otimes(\mathbf{b}\times\mathbf{c})\big)_{ij} = a_i\varepsilon_{jrq}b_rc_q$. The general conditions resulting from (11.8) are complicated and not at all transparent; for that reason we consider only the non-degenerate case in which $\{\mathbf{n}, \mathbf{m}^\varphi, \mathbf{m}^\kappa\}$ is linearly independent, so that

$$(\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi \neq 0. \qquad (11.9)$$

Since $(\mathbf{n}\times\mathbf{m}^\varphi)\cdot\mathbf{m}^\varphi = 0$, acting with (11.9) on $\mathbf{m}^\varphi$ yields

$$\big((\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi\big)\dot{\gamma}^\kappa\mathbf{s}^\kappa = \big((\mathbf{n}\times\mathbf{m}^{\bar{\varphi}})\cdot\mathbf{m}^\varphi\dot{\gamma}^{\bar{\varphi}}\big)\mathbf{s}^{\bar{\varphi}} + \big((\mathbf{n}\times\mathbf{m}^{\bar{\kappa}})\cdot\mathbf{m}^\varphi\big)\dot{\gamma}^{\bar{\kappa}}\mathbf{s}^{\bar{\kappa}}, \qquad (11.10)$$

which, upon dividing by $(\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi$ takes the form

$$\dot{\gamma}^\kappa\mathbf{s}^\kappa = \frac{(\mathbf{n}\times\mathbf{m}^{\bar{\varphi}})\cdot\mathbf{m}^\varphi}{(\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi}\dot{\gamma}^{\bar{\varphi}}\mathbf{s}^{\bar{\varphi}} + \frac{(\mathbf{n}\times\mathbf{m}^{\bar{\kappa}})\cdot\mathbf{m}^\varphi}{(\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi}\dot{\gamma}^{\bar{\kappa}}\mathbf{s}^{\bar{\kappa}}, \qquad (11.11)$$

Finally, taking the inner product of this relation with $\mathbf{s}^\kappa$ yields an equation for the slip $\dot{\gamma}^\kappa$, and interchanging the roles of φ and κ, we find that a relation for the slip $\dot{\gamma}^\varphi$; the results,

$$\left.\begin{aligned}\dot{\gamma}^\kappa &= \frac{(\mathbf{n}\times\mathbf{m}^{\bar{\varphi}})\cdot\mathbf{m}^\varphi}{(\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi}(\mathbf{s}^\kappa\cdot\mathbf{s}^{\bar{\varphi}})\dot{\gamma}^{\bar{\varphi}} + \frac{(\mathbf{n}\times\mathbf{m}^{\bar{\kappa}})\cdot\mathbf{m}^\varphi}{(\mathbf{n}\times\mathbf{m}^\kappa)\cdot\mathbf{m}^\varphi}(\mathbf{s}^\kappa\cdot\mathbf{s}^{\bar{\kappa}})\dot{\gamma}^{\bar{\kappa}},\\[2mm]\dot{\gamma}^\varphi &= \frac{(\mathbf{n}\times\mathbf{m}^{\bar{\varphi}})\cdot\mathbf{m}^\kappa}{(\mathbf{n}\times\mathbf{m}^\varphi)\cdot\mathbf{m}^\kappa}(\mathbf{s}^\varphi\cdot\mathbf{s}^{\bar{\varphi}})\dot{\gamma}^{\bar{\varphi}} + \frac{(\mathbf{n}\times\mathbf{m}^{\bar{\kappa}})\cdot\mathbf{m}^\kappa}{(\mathbf{n}\times\mathbf{m}^\varphi)\cdot\mathbf{m}^\kappa}(\mathbf{s}^\varphi\cdot\mathbf{s}^{\bar{\kappa}})\dot{\gamma}^{\bar{\kappa}},\end{aligned}\right\} \tag{11.12}$$

represent a pair of equations for the slips $\dot{\gamma}^\kappa$ and $\dot{\gamma}^\varphi$ in terms of the slips of the other grain. The existence of such transmission conditions would seem to lend credence to Conjecture ($*$).

11.2   Virtual power at the grain boundary. Force balances

Consider a part R (subregion of the bicrystal) that intersects the grain boundary. Then the external power expenditure for R has the form $(3.8)_2$, but the internal expenditure $(3.8)_1$ must be modified to account for power expenditures within the grain boundary. Basic to our theory is the presumption that *dissipation at the grain boundary arises as a consequence of an imbalance in the Burgers-vector flow across it.* Specifically, we allow for an *internal force* $\mathbf{K}$ distributed over $\mathcal{G}$, and we assume that $\mathbf{K}$ is power-conjugate to $[\![\dot{\mathbf{H}}^p]\!](\mathbf{n}\times)$. Thus, bearing in mind (3.8) and (3.16), we write the internal and external power expenditures for R in the form

$$\left.\begin{aligned}\mathcal{W}_{\text{int}}(R) &= \int_R \mathbf{T}:\dot{\mathbf{H}}^e\,dV + \sum_\alpha\int_R(\pi^\alpha\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla\dot{\gamma}^\alpha)\,dV + \int_{\mathcal{G}\cap R}\mathbf{K}:[\![\dot{\mathbf{H}}^p(\mathbf{n}\times)]\!]\,dA,\\[2mm]\mathcal{W}_{\text{ext}}(R) &= \int_{\partial R}\mathbf{T}\mathbf{n}\cdot\dot{\mathbf{u}}\,dA + \int_R\mathbf{f}\cdot\dot{\mathbf{u}}\,dV + \sum_\alpha\int_{\partial R}(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot{\gamma}^\alpha\,dA.\end{aligned}\right\} \tag{11.13}$$

We isolate the grain boundary by formally passing to the limit as R tends to an arbitrary subsurface $\mathcal{A}$ of $\mathcal{G}$. In such a limit the *volume* integrals vanish, while

$$\int_{\partial R}\mathbf{T}\mathbf{n}\cdot\dot{\mathbf{u}}\,dA \to \int_{\mathcal{A}}(\mathbf{T}_2\mathbf{n} + \mathbf{T}_1(-\mathbf{n}))\cdot\dot{\mathbf{u}}\,dA = \int_{\mathcal{A}}[\![\mathbf{T}\mathbf{n}]\!]\cdot\dot{\mathbf{u}}\,dA \tag{11.14}$$

and

$$\int_{\partial R}(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot{\gamma}^\alpha\,dA \to \int_{\mathcal{A}}[\![(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot{\gamma}^\alpha]\!]\,dA.$$

Thus the internal and external power expenditures for an arbitrary subsurface $\mathcal{A}$ of $\mathcal{G}$ have the form

$$\left.\begin{aligned}\mathcal{W}_{\text{int}}(\mathcal{A}) &= \int_{\mathcal{A}}\mathbf{K}:[\![\dot{\mathbf{H}}^p(\mathbf{n}\times)]\!]\,dA,\\[2mm]\mathcal{W}_{\text{ext}}(\mathcal{A}) &= \int_{\mathcal{A}}[\![\mathbf{T}\mathbf{n}]\!]\cdot\dot{\mathbf{u}}\,dA + \sum_\alpha\int_{\mathcal{A}}[\![(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot{\gamma}^\alpha]\!]\,dA.\end{aligned}\right\} \tag{11.15}$$

The internal and external *virtual* powers associated with (11.15) are obtained by replacing $\dot{\mathbf{u}}$ and $\dot{\gamma}^\alpha$ (for each α) by their virtual counterparts $\tilde{\mathbf{u}}$ and $\tilde{\gamma}^\alpha$, so that, for $i = 1, 2$, $\dot{\mathbf{H}}_i^p$ is replaced by

$$\tilde{\mathbf{H}}_i^p = \sum_\alpha \tilde{\gamma}_i^\alpha\,\mathbb{S}_i^\alpha. \tag{11.16}$$

The principle of virtual power for the grain boundary is the requirement that these virtual powers be equal for any subsurface $\mathcal{A}$ of $\mathcal{G}$ and all choices of the virtual fields. Taking the virtual slip-rates equal to zero yields the macroscopic traction condition

$$[\![\mathbf{T}]\!]\mathbf{n} = \mathbf{0}. \tag{11.17}$$

Next, by (2.8) and (11.16), for $i = 1, 2$,

$$\mathbf{K} : \big(\tilde{\mathbf{H}}_i^p(\mathbf{n}\times)\big) = \sum_\alpha \mathbf{K} : \big(\tilde{\gamma}_i^\alpha \mathbb{S}_i^\alpha(\mathbf{n}\times)\big) = -\sum_\alpha \tilde{\gamma}_i^\alpha \big(\mathbf{K}(\mathbf{n}\times)\big) : \mathbb{S}_i^\alpha;$$

(11.17) therefore renders the virtual-power principle of the form

$$\int_{\mathcal{A}} [\![(\boldsymbol{\xi}^\alpha \cdot \mathbf{n})\,\dot{\gamma}^\alpha]\!]\,dA = \sum_\alpha \int_{\mathcal{A}} \Big\{ \tilde{\gamma}_1^\alpha \big(\mathbf{K}(\mathbf{n}\times)\big) : \mathbb{S}_1^\alpha - \tilde{\gamma}_2^\alpha \big(\mathbf{K}(\mathbf{n}\times)\big) : \mathbb{S}_2^\alpha \Big\}\,dA.$$

Thus, since the subsurface $\mathcal{A}$ and the virtual slips are arbitrary, we are led to the *microscopic force balances for the grain boundary*:

$$\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n} = -\mathbb{S}_1^\alpha : \big(\mathbf{K}(\mathbf{n}\times)\big), \qquad \boldsymbol{\xi}_2^\alpha \cdot \mathbf{n} = -\mathbb{S}_2^\alpha : \big(\mathbf{K}(\mathbf{n}\times)\big), \tag{11.18}$$

or, equivalently,

$$(\xi_i^\alpha)_1 m_i = -(\mathbb{S}_{ij}^\alpha)_1 K_{ri}\varepsilon_{rkj} m_k, \qquad (\xi_i^\alpha)_2 m_i = -(\mathbb{S}_{ij}^\alpha)_2 K_{ri}\varepsilon_{rkj} m_k,$$

for each slip system α. Here, by (3.6),

$$\boldsymbol{\xi}_1^\alpha = \mathbf{m}_1^\alpha \times \mathbb{T}_1 \mathbf{s}_1^\alpha, \qquad \boldsymbol{\xi}_2^\alpha = \mathbf{m}_2^\alpha \times \mathbb{T}_2 \mathbf{s}_2^\alpha. \tag{11.19}$$

Note that, by (3.19), we can write the microforce balances in the form

$$\mathbb{S}_1^\alpha : \big(\mathbb{T}_1^\top(\mathbf{n}\times) + \mathbf{K}(\mathbf{n}\times)\big) = 0, \qquad \mathbb{S}_2^\alpha : \big(\mathbb{T}_2^\top(\mathbf{n}\times) + \mathbf{K}(\mathbf{n}\times)\big) = 0, \tag{11.20}$$

for each α. When the Schmid tensors span the space of deviatoric tensors, as is the case for FCC and BCC crystals (footnote 3), then, by (2.13), can rewrite the microforce balances in the form

$$\mathbb{T}_1^\top(\mathbf{n}\times) = -\mathbf{K}(\mathbf{n}\times), \qquad \mathbb{T}_2^\top(\mathbf{n}\times) = -\mathbf{K}(\mathbf{n}\times), \tag{11.21}$$

or, equivalently,

$$[\![\mathbb{T}^\top]\!](\mathbf{n}\times) = \mathbf{0}, \qquad \langle\!\langle \mathbb{T}^\top \rangle\!\rangle(\mathbf{n}\times) = -\mathbf{K}(\mathbf{n}\times). \tag{11.22}$$

The balances (11.22), in components, have the form

$$[\![\mathbb{T}_{rs}]\!]\varepsilon_{rkj} m_k = 0 \qquad \langle\!\langle T_{rs} \rangle\!\rangle\varepsilon_{rkj} m_k = -K_{rs}\varepsilon_{rkj} m_k.$$

11.3   Dissipation. Constitutive equation for the grain boundary

Dissipation inequality

We neglect the free energy of the grain boundary. The energy imbalance for the grain boundary, which is easily derived by applying, to (4.1), a limiting process similar to that leading to (11.15), has the simple form

$$\int_{\mathcal{A}} \mathbf{K} : [\![\dot{\mathbf{H}}^p(\mathbf{n}\times)]\!]\,dA \geq 0,$$

which localizes to

$$\mathcal{D} \overset{\text{def}}{=} \mathbf{K} : [\![\dot{\mathbf{H}}^p(\mathbf{n}\times)]\!] \geq 0; \tag{11.23}$$

$\mathcal{D}$ represents the *grain-boundary dissipation*, per unit area. Noting that the internal force $\mathbb{K}$ enters the balances (11.18), (11.20), and (11.22) through the term $\mathbb{K} : (\mathbf{n}\times)$, we use (2.9) to rewrite the dissipation in the form

$$\mathcal{D} = -\big(\mathbb{K}(\mathbf{n}\times)\big) : \big([\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big). \tag{11.24}$$

Constitutive equation for the grain boundary

We assume that *the processes under consideration begin from a virgin state*, so that, in particular,

$$\mathbf{H}^p(\mathbf{x}, 0) \equiv \mathbf{0}. \tag{11.25}$$

Then

$$\dot{H} \stackrel{\text{def}}{=} \big\| [\![\dot{\mathbf{H}}^p]\!](\mathbf{n}\times) \big\| = \big\| [\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n}) \big\| \tag{11.26}$$

(cf. (2.11)) is a measure of:

(i) the *impermeability* of $\mathcal{G}$ to Burgers-vector flow:

(ii) the *Burgers-vector production* within $\mathcal{G}$.

Further, H itself, which, by (11.25), is well defined, may be viewed as a measure of the *accumulated defectiveness* of $\mathcal{G}$. Guided by the dissipation inequality (11.24) and the foregoing discussion, we posit a viscoplastic constitutive relation for the grain boundary of the form

$$\mathbf{K}(\mathbf{n}\times) = -g(H, \dot{H}) \frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}, \tag{11.27}$$

where g is a scalar modulus assumed consistent with $g(H, \dot{H}) > 0$, $\dot{H} \neq 0$.[9] This constitutive choice is consistent with the dissipation inequality (11.24); in fact,

$$\mathcal{D} = g(H, \dot{H}) \big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|,$$

so that, by (2.12), $\mathbf{K}$ and (hence) the dissipation vanish whenever $\mathcal{G}$ is permeable to Burgers-vector flow.

11.4 Flow rule for the grain boundary

Combining the balances (11.18) with the constitutive equation (11.27), we arrive at a *flow rule* requiring that, for each slip system α,

$$\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n} = g(H, \dot{H}) \mathbb{S}_1^\alpha : \frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}, \qquad \boldsymbol{\xi}_2^\alpha \cdot \mathbf{n} = g(H, \dot{H}) \mathbb{S}_2^\alpha : \frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}. \tag{11.28}$$

When g has the power-law form

$$g(H, \dot{H}) = k_0(H)\, \dot{H}^\delta, \tag{11.29}$$

then (11.28) become

$$\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n} = k_0(H)\, \dot{H}^\delta\, \mathbb{S}_1^\alpha : \frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}, \qquad \boldsymbol{\xi}_2^\alpha \cdot \mathbf{n} = k_0(H)\, \dot{H}^\delta\, \mathbb{S}_2^\alpha : \frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}. \tag{11.30}$$

For δ small the flow rule (11.30) exhibit *small rate-dependences*.

For the remainder of this section we assume that

- *the Schmid tensors span the space of deviatoric tensors.*

The flow rule then consists of the balance $(11.22)_2$ supplemented by the constitutive equation (11.27),

$$\langle\!\langle \mathbb{T}^\top \rangle\!\rangle (\mathbf{n}\times) = g(H, \dot{H}) \frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}; \tag{11.31}$$

---

[9]One might also allow for dependences on the fields A_i defined by $\dot{A}_i = \big\|\dot{\mathbf{H}}_i^p(\mathbf{n}\times)\big\|$, which measure the accumulated Burgers vector in the individual grains at the grain boundary.

when g is given by the power law (11.29) this flow rule has the form

$$\langle\!\langle\mathbb{T}^\top\rangle\!\rangle(\mathbf{n}\times) = k_0(H)\,\dot{H}^\delta\,\frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}. \tag{11.32}$$

Since, by (2.11),

$$\big\|\langle\!\langle\mathbb{T}^\top\rangle\!\rangle(\mathbf{n}\times)\big\| = \big\|\langle\!\langle\mathbb{T}^\top\rangle\!\rangle\mathbb{P}(\mathbf{n})\big\| = \big\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbb{T}\rangle\!\rangle\big\|,$$

and since

$$\left\|\frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|}\right\| = 1,$$

(11.32) has the interesting consequence

$$\big\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbb{T}\rangle\!\rangle\big\| = k_0(H)\,\dot{H}^\delta. \tag{11.33}$$

When the behavior described by the flow rule (11.32) is *rate independent* as characterized by the limit $\delta \to 0$, then the condition $[\![\dot{\mathbf{H}}^p]\!](\mathbf{n}\times) = \mathbf{0}$ renders (11.32) meaningless, because then $[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n}) = \mathbf{0}$ and

$$\frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|} \tag{11.34}$$

is *undefined.* For that reason and because $\mathbf{K}$ is then absent from the dissipation inequality (11.23), *we consider the internal microforce* $\mathbf{K}$ *as indeterminate and, hence, do not require that* $\langle\!\langle\mathbb{T}^\top\rangle\!\rangle(\mathbf{n}\times)$ *be subject to a flow rule.* On the other hand, when $[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n}) \neq \mathbf{0}$, the flow rule

$$\langle\!\langle\mathbb{T}^\top\rangle\!\rangle(\mathbf{n}\times) = k_0(H)\frac{[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})}{\big\|[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})\big\|} \tag{11.35}$$

is to be satisfied, so that, as vectors in the space of deviatoric tensors, $\langle\!\langle\mathbb{T}^\top\rangle\!\rangle(\mathbf{n}\times)$ must be parallel to and point in the same direction as (11.34). Moreover, by (11.33), for $[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n}) \neq \mathbf{0}$,

$$\big\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbb{T}\rangle\!\rangle\big\| = k_0(H), \tag{11.36}$$

so that $k_0(H)$ represents the *grain-boundary flow stress*, and (11.34) must be normal to the *grain-boundary yield surface* represented by the sphere of radius $k_0(H)$ in the space of all tensors $\mathbf{A}\mathbb{P}(\mathbf{n})$ with $\mathbf{A}$ deviatoric.

Recall our assumption that the processes under consideration begin from a virgin state. Then, assuming that $\mathbb{T} = \mathbf{0}$ when $\mathbf{G} = \mathbf{0}$, there is an initial time interval during which

$$\big\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbb{T}\rangle\!\rangle\big\| < k_0(0). \tag{11.37}$$

During this time interval $[\![\dot{\mathbf{H}}^p]\!]\mathbb{P}(\mathbf{n})$ vanishes, so that $\mathcal{G}$ is permeable and, in view of the paragraph containing (11.7), $\mathcal{G}$ is defect-free. (Thus the set interior to the sphere of radius $k_0(H)$ bears comparison to the elastic range in the classical theory of plasticity, as both are defect free before initial yield.)

11.5 Qualitative behavior. Comparison with experiments

To discuss the qualitative behavior predicted by the theory, we allow for rate-dependent behavior, but with

$$\delta \approx 0,$$

and we restrict attention to monotone loading. We consider the simple defect energy $\Psi(\mathbf{G}) = \frac{1}{2}c\|\mathbf{G}\|^2$, $c > 0$, so that, by (5.6), $\mathbb{T} = c\mathbf{G}$ and the flow rule takes the form

$$\big\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbf{G}\rangle\!\rangle\big\| = k_1(H)\,\dot{H}^\delta, \qquad k_1(H) = \frac{k_0(H)}{c} > 0. \tag{11.38}$$

(a) Consider the initial stage of the loading. As there is a stress concentration at the grain boundary due to the mismatch in crystal orientations, large slip gradients should develop near the grain boundary, and this, in turn, should result in an increase in $\|\mathbf{G}\|$ near $\mathcal{G}$, but not away from $\mathcal{G}$, where one would expect $\|\mathbf{G}\|$ to be of lesser magnitude. Thus we would expect $\|\mathbf{G}\|$ to exhibit a sharp peak in each grain at $\mathcal{G}$. Moreover, since $\delta \approx 0$, the rate-independent theory should aproximate the rate-dependent theory and we may conclude from the paragraph containing (11.37) that there should be a nontrivial initial interval during which $\dot{H}$ is small and (hence) during which the grain boundary is approximately both permeable and defect free.

(b) By (11.38), as $\|\mathbf{G}\|$ increases at the grain boundary, so also should $\dot{H}$. But, because the relation (11.38) is exponential with exponent $\delta \approx 0$, $\dot{H}$ may attain large values with only minor changes in $\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbf{G}\rangle\!\rangle\|$. With increasing loading this relatively constant behavior of $\|\mathbb{P}(\mathbf{n})\langle\!\langle\mathbf{G}\rangle\!\rangle\|$ would tend to (at least in part) hold $\|\mathbb{P}(\mathbf{n})\mathbf{G}^{\pm}\|$ nearly constant; in fact, if the hardening function $k_0(H)$ ultimately decreases with H, then $\|\mathbb{P}(\mathbf{n})\mathbf{G}^{\pm}\|$ should ultimately *decrease*. Moreover, experience with more classical plasticity theories based on a power law with small exponent would seem to imply that the transition from the behavior specified in (a) should be sharp.

(c) Summarizing, for a bicrystal under monotone loading from a virgin state, there should be an initial loading interval during which a sharp peak $\|\mathbf{G}\|$ develops on the two sides of the grain boundary and during which the grain boundary is approximately both permeable and defect free. Then, following a sharp transition, $\|\mathbb{P}(\mathbf{n})\mathbf{G}^{\pm}\|$ should not vary appreciably.

The behavior summarized in (c), which is a consequence of the grain-boundary flow rule (11.32), seems consistent with experiments of Sun et al. (1998, 2000), who determine the Burgers tensor in an Al bicrystal through measurements of lattice rotations. These experiments show an ultimate strain softening at the grain boundary, behavior easily accomodated within our theory by allowing $k_0(H)$ to ultimately decrease with H. Finite element calculations based on conventional single-crystal plasticity reported in Sun et al. (2000) predict that the sharp peak $\|\mathbf{G}\|$ on the two sides of the grain boundary persists at large strains, in disagreement with the experiments. What seems to be missing from conventional theory is that the increased Burgers-vector magnitude in the boundary layer can promote nucleation of slip, so that, effectively, the grain boundary softens. The framework here allows for such softening. Finally, the calculations agree fairly well with the experiments at 10% strain, which would seem consistent with the ultimate assertion in (a), granted our conjecture stated on page 19 is correct.

References

ASARO, R. J. RICE, J. R., 1977. Strain localization in ductile single crystals. *Journal of the Mechanics and Physics of Solids* **25**, 309-338.

BITTENCOURT, E. NEEDLEMAN, A. VAN DER GIESSEN, E. GURTIN, M. E., 2003, A comparison of nonlocal continuum and discrete dislocation plasticity predictions, *Journal of the Mechanics and Physics of Solids*, **51**, 281-310

BURGERS, J. M., 1939. Some considerations of the field of stress connected with dislocations in a regular crystal lattice, *Koninklijke Nederlandse Akademie van Wetenschappen*, **42**, 293-325 (Part 1) 378-399 (Part 2).

CERMELLLI. P. GURTIN, M. E., 2002, Geometrically necessary dislocations in viscoplastic single crystals and bicrystals undergoing small deformations, *International Journal of Solids and Structures*, **39**, 6281-6309.

CLEVERINGA, H. H. M. VAN DER GIESSEN, E. NEEDLEMAN, A., 1999. A discrete dislocation analysis of residual stresses in a composite material. *Philosophcal Magazine A*, **79**, 893-920.

FLECK, N. A. MULLER, G. M. ASHBY, M. F. HUTCHINSON, J. W., 1994. Strain gradient plasticity: theory and experiment. *Acta metallurgica* **42**, 475-487.

GURTIN, M. E., 2002. A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations. *Journal of the Mechanics and Physics of Solids*, **50**, 5-32.

HILL R. RICE, J. R., 1972. Constitutive analysis of elastic-plastic crystals at arbitrary strain. *Journal of the Mechanics and Physics of Solids* **20**, 401-413.

KRÖNER, E., 1960. Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen, *Archive for Rational Mechanics and Analysis* **4**, 273–334.

MANDEL, J., 1965. Generalisation de la theorie de la plasticite de W. T. Koiter. *International Journal of Solids and Structures* **1**, 273-295.

RICE, J. R., 1971. Inelastic constitutive relations for solids: an internal-variable theory and its applications to metal plasticity. *Journal of the Mechanics and Physics of Solids* **19**, 443-455.

SUN, S. ADAMS, B. L. SHET, C. Q SAIGAL, S. KING, W., 1998. Mesoscale investigation of the deformation field of an aluminum bicrystal, *Scripta Materialia* **39**, 501-508.

SUN, S. ADAMS, B. L. KING, W., 2000. Observations of lattice curvature near the interface of a deformed aluminium bicrystal. *Philosophical Magazine A* , **80**, 9-25.

TAYLOR, G. I. ELAM, C. F., 1923. The distortion of an aluminum crystal during a tensile test. *Proceedings of the Royal Society of London* **102A**, 643-667.

TAYLOR, G. I. ELAM, C. F., 1925. The plastic extension and fracture of aluminum crystals. *Proceedings of the Royal Society of London* **108A**, 28-51.

TAYLOR, G. I., 1938a. Plastic strain in metals. *Journal of the Institute of Metals* **62**, 307-325.

TAYLOR, G. I., 1938b. Analysis of plastic strain in a cubic crystal. In: Lessels, J. M. (Ed.), *Stephen Timoshenko Anniversary Volume*. Macmillan, New York.