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# Geometrically necessary dislocations in viscoplastic single crystals and bicrystals undergoing small deformations

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**Abstract**

In this study we develop a gradient theory of small-deformation single-crystal plasticity that accounts for geometrically necessary dislocations (GNDs). The resulting framework is used to discuss grain boundaries. The grains are allowed to slip along the interface, but growth phenomenona and phase transitions are neglected. The bulk theory is based on the introduction of a microforce balance for each slip system and includes a *defect energy* depending on a suitable measure of GNDs. The microforce balances are shown to be equivalent to *nonlocal* yield conditions for the individual slip systems, yield conditions that feature backstresses resulting from energy stored in dislocations. When applied to a grain boundary the theory leads to concomitant yield conditions: relative slip of the grains is activated when the shear stress reaches a suitable threshold; plastic slip in bulk at the grain boundary is activated only when the local density of GNDs reaches an assigned threshold. Consequently, in the initial stages of plastic deformation the grain boundary acts as a barrier to plastic slip, while in later stages the interface acts as a source or sink for dislocations. We obtain an exact solution for a simple problem in plane strain involving a semi-infinite compressed specimen that abuts a rigid material. We view this problem as an approximation to a situation involving a grain boundary between a grain with slip systems aligned for easy flow and a grain whose slip system alignment severely inhibits flow. The solution exhibits large slip gradients within a thin layer at the grain boundary.



*Keywords:* Dislocations; Grain boundaries; Crystal plasticity; Nonlocal plasticity

## 1. Introduction

This paper has two goals. The first is a generalization of classical single crystal, small-deformation viscoplasticity [1] that accounts for geometrically necessary dislocations, here referred to as GNDs. This

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[1] Cf. Mandel (1965), Rice (1971), Hill and Rice (1972), Teodosiu and Sidoroff (1976), Asaro and Rice (1977), Asaro (1983a,b), Asaro and Needleman (1985) and Bronkhorst et al. (1992). See also Taylor and Elam (1923, 1925) and Taylor (1938a,b). The extreme sensitivity of single-crystal plasticity to the presence of GNDs is underlined in the discrete-dislocation analysis of Cleveringa et al. (1999).



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generalization—formulated in terms of a microscopic balance involving forces work conjugate to slip in conjunction with the kinematics of GNDs (Burgers, 1939; Kröner, 1960)—is based on and follows closely its finite deformational counterpart developed by Gurtin (2002).

Our second goal, which builds on the single-crystal theory discussed above, is a theory of bicrystals. Here our use of microforces equipped with their peculiar balance allows for a direct characterization of grain boundaries based on physical quantities associated directly with the individual slip systems.

### 1.1. Classical single-crystal viscoplasticity

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. The classical theory of plasticity is based on the decomposition [2]

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

in which $\mathbf{H}^e$ represents stretching and rotation of the *lattice*, while $\mathbf{H}^p$ represents the evolution of dislocations through the lattice. The symmetric and skew parts of $\mathbf{H}^e$, namely

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

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

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

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 *kinematic constitutive assumption*

$$\mathbf{H}^p = \sum_{\alpha=1}^{A} \gamma^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha. \tag{1.4}$$

Here and in what follows, lower case Greek superscripts $\alpha, \beta, \ldots$ denote slip-system labels and as such have the range $1, 2, \ldots, A$. In the absence of work hardening the classical theory is typically based on viscoplastic yield conditions

$$\tau^\alpha = \sigma^\alpha |\dot{\gamma}^\alpha|^\delta \operatorname{sgn} \dot{\gamma}^\alpha. \tag{1.5}$$

Here $\tau^\alpha$, the resolved shear, is the macroscopic stress resolved on the $\alpha$th slip system; the field $\sigma^\alpha > 0$, the *slip resistance* on $\alpha$, is an internal state-variable consistent with a system of *hardening equations*

$$\dot{\sigma}^\alpha = \sum_{\beta=1}^{A} k^{\alpha\beta}(\sigma^1, \sigma^2, \ldots, \sigma^A)|\dot{\gamma}^\beta|, \qquad \sigma^\alpha(\mathbf{x},0) = \sigma_0^\alpha > 0, \tag{1.6}$$

where the moduli $k^{\alpha\beta} \geqslant 0$ characterize strain-hardening due to slip; and $\delta > 0$ is a constant that characterizes the rate dependence of the material. [3] These equations supplemented by the local momentum balance and a standard elastic stress–strain relation form the basic equations of the theory.

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[2] We use lightface for *scalars* $(a, b, A, \ldots)$; lower-case boldface for *vectors* $(\mathbf{a}, \mathbf{b}, \ldots)$; upper-case boldface for *tensors* $(\mathbf{E}, \mathbf{T}, \ldots)$. We write $\operatorname{tr}\mathbf{T}$ and $\mathbf{T}^\top$ for the *trace and transpose* of a (second-order) tensor $\mathbf{T}$ and use a "dot" to denote the inner product of tensors: $\mathbf{T}\cdot\mathbf{E} = T_{ij}E_{ij}$ (using cartesian components and summation convention). Given any vector $\mathbf{u}$, $(\mathbf{u}\times)$ is the *skew tensor* defined by $(\mathbf{u}\times)_{ij} = \varepsilon_{irj}u_r$. For $\mathbf{C}$ a fourth-order tensor and $\mathbf{E}$ a second-order tensor, $(\mathbf{C}[\mathbf{E}])_{ij} = C_{ijkl}E_{kl}$. For $\mathbf{u}$ a vector field and $\mathbf{T}$ a tensor field, $(\nabla\mathbf{u})_{ij} = \partial u_i/\partial x_j$, $(\operatorname{div}\mathbf{T})_i = \partial T_{ij}/\partial x_j$, and $(\operatorname{curl}\mathbf{T})_{ij} = \varepsilon_{ipq}\partial T_{jq}/\partial x_p$.

[3] Most metals at room temperature are almost rate independent and as such would be described by small values of $\delta$.

### 1.2. Generalization of the classical theory: a gradient theory that accounts for GNDs

The plastic distortion $\mathbf{H}^p$ is not the gradient of a vector field, and GNDs may be characterized by the closure failure of circuits as mapped by $\mathbf{H}^p$, and hence by the *geometric dislocation tensor*

$$\mathbf{G} = \operatorname{curl}\mathbf{H}^p. \tag{1.7}$$

Here we generalize the classical theory by allowing for constitutive dependences on $\mathbf{G}$. We accomplish this by developing the theory within a framework that allows for microforces whose working accompanies slip as described by the fields $\gamma^\alpha$. This microforce system consists of *vector* stresses $\boldsymbol{\xi}^\alpha$ and *scalar* internal forces $\pi^\alpha$ whose working, *within* any subbody $R$, is given by

$$\sum_{\alpha=1}^{A}\int_R (\pi^\alpha\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla\dot{\gamma}^\alpha)\,\mathrm{d}V.$$

Because of the nonstandard nature of the microforces, we base our treatment on the principle of virtual power. A consequence of this principle is that the classical Newtonian balances need be supplemented by a *microforce balance*

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

for each slip-system $\alpha$ (Gurtin, 2000). The presence of the resolved shear $\tau^\alpha$ couples the macroscopic and microscopic systems.

We restrict attention to a purely mechanical theory with underlying "second law" the requirement that the free-energy increase at a rate not greater than the rate at which work is performed. Letting $\psi$ denote the *free energy* per unit volume and $\mathbf{T}$ the stress, this leads to a local free-energy inequality

$$\dot{\psi} - \mathbf{T}\cdot\dot{\mathbf{E}}^e - \sum_{\alpha=1}^{A}(\boldsymbol{\xi}^\alpha\cdot\nabla\dot{\gamma}^\alpha + \pi^\alpha\dot{\gamma}^\alpha) \leqslant 0 \tag{1.8}$$

that is basic to our development of constitutive equations.

The classical theory fits trivially within this framework. To see this, assume that the free energy is "elastic", so that $\dot{\psi} = \mathbf{T}\cdot\dot{\mathbf{E}}^e$, take $\boldsymbol{\xi}^\alpha \equiv 0$, and define $\pi^\alpha = \sigma^\alpha|\dot{\gamma}^\alpha|^\delta \operatorname{sgn}\dot{\gamma}^\alpha$. The microforce balances $\tau^\alpha = \pi^\alpha$ are then satisfied trivially, as is the free-energy inequality. For the classical theory the additional structure represented by the microforce balances and second law is of little benefit. But the inclusion of GNDs leads to a gradient theory, and here the microforce balances and second law yield a physical framework that accounts in a natural manner for the distribution of GNDs within the body.

To develop a crystalline theory that accounts for GNDs, we take a physical approach that underlines the reasons for specific constitutive assumptions:

(i) We model distortions of the crystal lattice due to GNDs by augmenting the classical quadratic strain energy with a defect energy $\Psi(\mathbf{G})$. [4]
(ii) Using the free-energy inequality as a guide, we develop appropriate constitutive equations for the microforce fields. The microforce balances and these constitutive equations together form the viscoplastic yield conditions.

In appealing to the free-energy inequality we do not seek the most general possible theory, but one with dissipative part close to its classical counterpart. In this spirit, we are led to constitutive equations for $\pi^\alpha$ and $\boldsymbol{\xi}^\alpha$, which, when substituted into the microforce balance, result in the *viscoplastic yield conditions*

[4] A free energy of this form was introduced by Teodosiu (1970) within a classical framework involving only standard forces.

$$\tau^\alpha = \sigma^\alpha f(\dot{\gamma}^\alpha) - \mathrm{div}(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha), \quad \mathbb{T} = \partial\Psi/\partial\mathbf{G}. \tag{1.9}$$

Here $\sigma^\alpha f(\dot{\gamma}^\alpha)$, with $\sigma^\alpha$ consistent with the hardening equations (1.6) and $f$, possibly of the classical form

$$f(\dot{\gamma}^\alpha) = |\dot{\gamma}^\alpha|^\delta \,\mathrm{sgn}\,\dot{\gamma}^\alpha, \tag{1.10}$$

is *dissipative*, while

$$\mathrm{div}(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) \tag{1.11}$$

is *strictly energetic*. The term (1.11) is characteristic of kinematic hardening; its negative represents a *backstress on the* $\alpha$*th slip system* (cf. the discrete-dislocation computations of Cleveringa et al. (1999), which display large backstresses).

The chief conceptual difference between the classical theory and that presented here is that the yield conditions (1.9) represent constitutively augmented microscopic force balances. This difference renders the yield conditions nonlocal (in fact, dependent on first and second slip-gradients) and suggests the need for supplementary boundary conditions; we here discuss idealized boundary conditions that represent microscopic counterparts of clamped and free boundaries. Because the underlying mechanics is based on the principle of virtual power, the yield conditions and microtraction boundary conditions have a variational formulation (cf. Gurtin, 2002) that should provide a useful basis for computations. The theory presented here, which is the small-deformation counterpart of the finite-deformation theory of Gurtin (2002), differs radically from other gradient theories of plasticity, [5] chiefly because of the central role played by the microforces and their abstract introduction as forces work conjugate to slip. For that reason, we sketch an argument of Gurtin (2002) showing that the microstresses $\boldsymbol{\xi}^\alpha$ represent counterparts within the present theory of the classical *Peach–Koehler force* on a single dislocation.

### *1.3. Bicrystals: theory without interfacial energy*

Grain boundaries influence the plastic behavior of polycrystalline solids in many ways: (i) they modify the yield stress of the material, acting as barriers for glide dislocations in the initial stages of plastic deformation (cf. e.g., Hirth, 1972; Miracle, 1991; Mandal and Baker, 1995; François et al., 1998; Polcarova et al., 1998); (ii) they may, conversely, act as sources of bulk dislocations, and thus transmit plastic slip between adjacent grains (Shen et al., 1988; Clark et al., 1991; Pestman and De Hosson, 1992); (iii) they may also promote superplastic behavior by a macroscopic slip mechanism: the grains may slip one relative to the other along the grain boundaries, and this may greatly enhance plastic deformation (see for instance Margolin (1998) and Fu et al. (2001)); (iv) grain boundaries may also act as channels for mass and impurity diffusion, or as nucleation or segregation sites for impurities or new-phase particles (François et al., 1998).

We focus here on the influence of grain boundaries on the evolution of GNDs in the interior of the grains, explicitly accounting for the barrier-effect on plastic slip.

The basic grain boundary relations that we obtain play the role of interfacial yield conditions. Specifically: (i) the relative slip of the grains along the boundary is activated when the shear stress at the interface reaches a suitable threshold; (ii) analogously, plastic slip within each grain at the grain boundary $S$ is

[5] Cf. Fleck and Hutchinson (1993) and Fleck et al. (1994), who develop small-strain theories that account for strain gradients within a Toupin-Mindlin framework; this work is reformulated by Fleck and Hutchinson (2001) using microforces. Cf. also Naghdi and Srinivasa (1993, 1994), who develop a finite Cosserat theory with GNDs characterized by $\mathrm{curl}\,\mathbf{F}^p$ (cf. Shizawa and Zbib, 1999). Earlier attempts are those of Aifantis (1984, 1987), Wright and Batra (1987), Batra (1987), Batra and Kim (1988), Muhlhaus and Aifantis (1991a,b), Zbib and Aifantis (1992). A survey of gradient plasticity theories is contained in the review of Fleck and Hutchinson (1997). The theories mentioned above all involve higher-order boundary conditions. A discussion of gradient theories not equipped with higher-order boundary conditions is beyond the present scope.

allowed on any given slip system $\alpha$ only when the component of the microstress $\boldsymbol{\xi}^\alpha$ normal to $S$ reaches an assigned threshold, thereby rendering the grain boundaries barriers to plastic slip in the initial stages of plastic deformation. [6]

Precisely, we consider a body composed of two grains, labelled by the integers 1, 2. Let $S$ denote the smooth surface that represents the *grain boundary*, and denote by $\mathbf{n}_S$ the unit normal to $S$ directed outward from grain 1. We assume that the grains are rotated one relative to the other, and write

$$\mathbf{s}_2^\alpha = \mathbf{R}\mathbf{s}_1^\alpha, \quad \mathbf{m}_2^\alpha = \mathbf{R}\mathbf{m}_1^\alpha, \tag{1.12}$$

where $\mathbf{R}$ is an assigned rotation, and $(\mathbf{s}_1^\alpha, \mathbf{m}_1^\alpha)$ and $(\mathbf{s}_2^\alpha, \mathbf{m}_2^\alpha)$ are the slip systems in grains 1 and 2, respectively. We allow the grains to slip, one relative to the other, along $S$, so that the displacement $\mathbf{u}$ may be discontinuous across $S$. We write $[\![\mathbf{u}]\!]$ for the jump [7] of $\mathbf{u}$ across $S$ and

$$\mathbf{d} = [\![\dot{\mathbf{u}}]\!]$$

for the *grain-boundary slip-rate*.

The first set of conditions at $S$ consists of the classical traction balance

$$[\![\mathbf{T}]\!]\mathbf{n}_S = \mathbf{0}$$

across $S$ in conjunction with a balance between the tangential tractions and the *grain-boundary shear-stress* $\boldsymbol{\tau}$:

$$(\mathbf{T}_1\mathbf{n}_S)_{\tan} = (\mathbf{T}_2\mathbf{n}_S)_{\tan} = \boldsymbol{\tau}.$$

Here $(\mathbf{T}_i\mathbf{n}_S)_{\tan}$ denotes the tangential projection of $\mathbf{T}_i\mathbf{n}_S$ on $S$. We consider a simple constitutive equation for $\boldsymbol{\tau}$ of the form [8]

$$\boldsymbol{\tau} = \varphi|\mathbf{d}|^\delta \frac{\mathbf{d}}{|\mathbf{d}|}. \tag{1.13}$$

Here $\varphi$ is a positive modulus. As suggested by experiment (Biscondi, 1982), $\varphi$ should depend on the orientation $\mathbf{n}_S$ of the boundary and the misorientation $\mathbf{R}$ of the grains. Choosing $\delta = 0$, the macroscopic slip condition (1.13) is rate independent and represents a Coulomb-friction law for the relative slip of the grains at the interface.

The second set of conditions at $S$ have the form of viscoplastic boundary conditions for the microforces $\boldsymbol{\xi}^\alpha$; viz.

$$\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n}_S = -\zeta_1^\alpha|\dot{\gamma}_1^\alpha|^\delta \operatorname{sgn}\dot{\gamma}_1^\alpha, \qquad \boldsymbol{\xi}_2^\alpha \cdot \mathbf{n}_S = \zeta_2^\alpha|\dot{\gamma}_2^\alpha|^\delta \operatorname{sgn}\dot{\gamma}_2^\alpha, \tag{1.14}$$

with the $\zeta_i^\alpha$ positive moduli that measure the resistence of the grain boundary to plastic slip. These moduli depend on the slip system under consideration, the orientation of the boundary with respect to the grains, the relative misorientation of the grains, and the net accumulated slip from both grains at the grain boundary (cf. (10.15) and (10.16)).

[6] These boundary conditions should be compared to those of Shu and Fleck (1999), who discuss bicrystals within the Fleck and Hutchinson (1997) theory. For grain-boundary conditions these authors augment more or less standard conditions with the requirement that the normal gradient of the displacement be continuous.

[7] We write $\varphi_1$ for the limit of a bulk field $\varphi$ at $S$ from grain 1, $\varphi_2$ for the limit from grain 2, and $[\![\varphi]\!] = \varphi_2 - \varphi_1$.

[8] Since slip across a grain boundary is generally a high temperature phenomenon, the condition (1.13) may be replaced by continuity of the displacement across $S$ under normal operating conditions (John Hutchinson, private communication). For convenience, we use the same power $\delta$ in all power laws.

Since the microstress $\boldsymbol{\xi}^\alpha$ is a function of the geometric dislocation tensor through the relation $\boldsymbol{\xi}^\alpha = \mathbf{m}^\alpha \times (\partial\Psi/\partial\mathbf{G})\mathbf{s}^\alpha$, the viscoplastic yield conditions (1.14) (with $\zeta_i^\alpha$ constant for the purpose of this discussion) may be interpreted as follows for a body under monotone increasing loading:

(a) In the initial stages of deformation, where the density of GNDs is small, the microtraction $\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n}_S$ on, say, the grain 1 side of $S$, should also be small and, by (1.14) and the assumption that the exponent $\delta$ is small, the slip-rate $\dot{\gamma}_1^\alpha \approx 0$. Thus in this regime, the grain boundary acts as a *barrier* for plastic slip. This constraint should induce increasing slip gradients on $\alpha$ near $S$ and this in turn should result in an increase in the density of GNDs at $S$ in grain 1. This should be a "boundary layer effect", not apparent away from $S$, where one would expect the accumulation of GND to be of lesser magnitude. Thus we would expect the dislocation content to exhibit a sharp peak at $S$ during the initial stages of flow.

(b) As the density of GNDs increases at the grain boundary, the microtraction $\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n}_S$ also increases, and this, by (1.14), eventually decrease the magnitude of the constraint on $\dot{\gamma}_1^\alpha$, which may attain large values with only minor changes in the microtraction $\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n}_S$. With increasing loading this relatively constant behavior of $\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n}_S$ would, since $\boldsymbol{\xi}^\alpha = \boldsymbol{\xi}^\alpha(\mathbf{G})$, tend to (at least in part) hold the content of GNDs at $S$ in grain 1 constant, especially if many slip systems are active there.

The behavior specified in (a) and (b), which is a consequence of the microtraction conditions at the grain boundary, seems consistent with the experiments of Sun et al. (1998, 2000), who determine the geometric dislocation tensor in a bicrystal through measurements of lattice rotations.

We discuss the specialization of the theory to strict plane strain, as the results there are more transparent. In particular, restricting attention to the rate-independent limit of the theory, we establish a more precise version of the remarks (a) and (b).

Finally, we obtain an exact solution of a simple problem in plane-strain involving a semi-infinite compressed specimen that abuts a rigid material. The solution may be viewed as an approximation to a situation involving a grain boundary between a grain with slip systems aligned for easy flow and a grain whose slip system alignment severely inhibits flow.

## 2. The geometric dislocation tensor G

### 2.1. *G in terms of slip gradients*

We base the theory on standard crystalline kinematics as specified in Section 1.1 with GNDs characterized by the geometric dislocation tensor as defined in (1.7). Since $\operatorname{curl}\nabla\mathbf{u} = \mathbf{0}$, we may use (1.1) to express $\mathbf{G}$ in terms of either $\mathbf{H}^e$ or $\mathbf{H}^p$:

$$\mathbf{G} = \operatorname{curl}\mathbf{H}^p = -\operatorname{curl}\mathbf{H}^e. \tag{2.1}$$

Further, since

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

(1.4) yields

$$\mathbf{G} = \sum_{\alpha=1}^{A}(\nabla\gamma^\alpha \times \mathbf{m}^\alpha) \otimes \mathbf{s}^\alpha. \tag{2.2}$$

Let $\partial S$ denote the boundary curve of an oriented plane surface $S$ with unit normal $\mathbf{e}$. By Stokes' theorem, the Burgers vector corresponding to the curve $\partial S$ is given by

$$\int_{\partial S}\mathbf{H}^p\,\mathrm{d}\mathbf{x} = \int_S (\operatorname{curl}\mathbf{H}^p)^{\mathsf{T}}\mathbf{e}\,\mathrm{d}A = \int_S \mathbf{G}^{\mathsf{T}}\mathbf{e}\,\mathrm{d}A. \tag{2.3}$$

The vector field $\mathbf{G}^{\mathsf{T}}\mathbf{e}$ therefore represents the *Burgers vector* (per unit area) for small loops on the plane $\Pi$ with unit normal $\mathbf{e}$; i.e., the local Burgers vector for those dislocation lines piercing $\Pi$.

### 2.2. Digression: G in terms of dislocation densities

Tensors such as $\mathbf{G}$ meant to characterize specific distributions of dislocations are often expressed as linear combinations of *dislocations* $\rho\boldsymbol{l}\otimes\mathbf{s}$. Here $\rho$ is a (signed) *density*, $\boldsymbol{l}\otimes\mathbf{s}$ is a *dislocation dyad*, and $\boldsymbol{l}$ and $\mathbf{s}$ are *unit vectors* with $\mathbf{s}$ the *Burgers direction* and $\boldsymbol{l}$ the *line direction* (Nye, 1953). Moreover, an *edge dislocation* has $\boldsymbol{l}\perp\mathbf{s}$, a *screw dislocation* has $\boldsymbol{l}=\mathbf{s}$, and a *mixed dislocation* has $\boldsymbol{l}$ and $\mathbf{s}$ neither parallel nor orthogonal.

A class of expansions in terms of dislocations consistent with the crystalline structure of the material was utilized by Kubin et al. (1992), Sun et al. (1998, 2000), and Arsenlis and Parks (1999), who note that *canonical dislocations for slip* on the $\alpha$th system are: screw dislocations with Burgers direction $\mathbf{s}^\alpha$; and edge dislocations with Burgers direction $\mathbf{s}^\alpha$ and line direction

$$\boldsymbol{l}^\alpha=\mathbf{m}^\alpha\times\mathbf{s}^\alpha.$$

The *canonical dislocation dyads* for slip on $\alpha$ are therefore $\mathbf{s}^\alpha\otimes\mathbf{s}^\alpha$ and $\boldsymbol{l}^\alpha\otimes\mathbf{s}^\alpha$, and Arsenlis and Parks (1999) have shown that the expression (2.2) may be rewritten as a decomposition of $\mathbf{G}$ in terms of such dyads; using "$\odot$" and "$\vdash$" as screw and edge symbols, this expansion has the form

$$\mathbf{G}=\sum_{\alpha=1}^{A}(\underbrace{\rho_\odot^\alpha\mathbf{s}^\alpha\otimes\mathbf{s}^\alpha}_{\text{pure screw dislocation}}+\underbrace{\rho_\vdash^\alpha\boldsymbol{l}^\alpha\otimes\mathbf{s}^\alpha}_{\text{pure edge dislocation}}),\quad \rho_\vdash^\alpha=-\mathbf{s}^\alpha\cdot\nabla\gamma^\alpha,\quad \rho_\odot^\alpha=\boldsymbol{l}^\alpha\cdot\nabla\gamma^\alpha. \tag{2.4}$$

Note that in each case *the directional derivative that defines the density is in a direction perpendicular to the line direction*.

To verify (2.4), fix $\alpha$, expand $\nabla\gamma^\alpha$ with respect to $\{\mathbf{s}^\alpha,\boldsymbol{l}^\alpha,\mathbf{m}^\alpha\}$, and then compute $\nabla\gamma^\alpha\times\mathbf{m}^\alpha$; the result is

$$(\mathbf{s}^\alpha\cdot\nabla\gamma^\alpha)(\mathbf{s}^\alpha\times\mathbf{m}^\alpha)+(\boldsymbol{l}^\alpha\cdot\nabla\gamma^\alpha)(\boldsymbol{l}^\alpha\times\mathbf{m}^\alpha)=-(\mathbf{s}^\alpha\cdot\nabla\gamma^\alpha)\boldsymbol{l}^\alpha+(\boldsymbol{l}^\alpha\cdot\nabla\gamma^\alpha)\mathbf{s}^\alpha.$$

Thus

$$(\nabla\gamma^\alpha\times\mathbf{m}^\alpha)\otimes\mathbf{s}^\alpha=-(\mathbf{s}^\alpha\cdot\nabla\gamma^\alpha)\boldsymbol{l}^\alpha\otimes\mathbf{s}^\alpha+(\boldsymbol{l}^\alpha\cdot\nabla\gamma^\alpha)\mathbf{s}^\alpha\otimes\mathbf{s}^\alpha$$

and (2.2) reduces to (2.4).

## 3. Principle of virtual power—macroscopic and microscopic force balances

We write

$$\boldsymbol{\gamma}=(\gamma^1,\gamma^2,\dots,\gamma^A)$$

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

$$\nabla\dot{\mathbf{u}}=\dot{\mathbf{E}}^e+\dot{\mathbf{W}}^e+\sum_{\alpha=1}^{A}\dot{\gamma}^\alpha(\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha) \tag{3.1}$$

(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

With each evolution of the body we associate macroscopic and microscopic force systems. The macroscopic system is defined by a *traction* $\mathbf{t}(\mathbf{n})$ (for each unit vector $\mathbf{n}$), a field with a more or less standard interpretation, and an external *body force* $\mathbf{f}$ presumed to *account for inertia*. The microscopic system, which is nonstandard, is defined by: (i) a *lattice stress* $\mathbf{T}$ that expends power over the lattice strain-rate $\dot{\mathbf{E}}^e$; (ii) an *internal microforce* $\pi^\alpha$ for each slip system $\alpha$ that expends power over the slip-rate $\dot{\gamma}^\alpha$; (iii) a *microstress* $\boldsymbol{\xi}^\alpha$ that expends power over the slip-rate gradient $\nabla\dot{\gamma}^\alpha$; and (iv) a *microtraction* $\Xi^\alpha(\mathbf{n})$ that expends power over $\dot{\gamma}^\alpha$. Since $\dot{\mathbf{E}}^e$ is symmetric, we require that the lattice stress $\mathbf{T}$ be *symmetric*.

We characterize the force systems through the manner in which they expend power; that is, given any subbody $R$, through the specification of: (i) $\mathscr{P}_{\rm ext}(R)$, the power expended on $R$ by material *external* to $R$; and (ii) $\mathscr{P}_{\rm int}(R)$, a concomitant expenditure of power *within* $R$. Precisely,

$$\left.\begin{aligned}\mathscr{P}_{\rm ext}(R) &= \textstyle\int_{\partial R}\mathbf{t}(\mathbf{n})\cdot\dot{\mathbf{u}}\,\mathrm{d}A + \int_R \mathbf{f}\cdot\dot{\mathbf{u}}\,\mathrm{d}V + \sum_{\alpha=1}^{A}\int_{\partial R}\Xi^\alpha(\mathbf{n})\dot{\gamma}^\alpha\,\mathrm{d}A,\\ \mathscr{P}_{\rm int}(R) &= \textstyle\int_R \mathbf{T}\cdot\dot{\mathbf{E}}^e\,\mathrm{d}V + \sum_{\alpha=1}^{A}\int_R(\pi^\alpha\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla\dot{\gamma}^\alpha)\,\mathrm{d}V.\end{aligned}\right\} \tag{3.2}$$

Fix the time and consider the fields $\dot{\mathbf{u}}$, $\dot{\mathbf{E}}^e$, 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 $\tilde{\mathbf{u}}$, $\widetilde{\mathbf{E}}^e$, and $\tilde{\boldsymbol{\gamma}}$ to distinguish them from fields associated with the actual evolution of the body, we require that

$$\nabla\tilde{\mathbf{u}} = \widetilde{\mathbf{E}}^e + \widetilde{\mathbf{W}}^e + \sum_{\alpha=1}^{A}\tilde{\gamma}^\alpha(\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha) \tag{3.3}$$

for some *skew* tensor field $\widetilde{\mathbf{W}}^e$. Further, we define a *generalized virtual velocity* to be a list

$$\mathscr{V} = (\tilde{\mathbf{u}}, \widetilde{\mathbf{E}}^e, \tilde{\boldsymbol{\gamma}})$$

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

We postulate a *principle of virtual power* requiring that, given any generalized virtual velocity $\mathscr{V}$ and any subbody $R$, the corresponding internal and external virtual powers are balanced:

$$\mathscr{P}_{\rm ext}(R,\mathscr{V}) = \mathscr{P}_{\rm int}(R,\mathscr{V}). \tag{3.4}$$

### 3.2. Macroscopic and microscopic force balance

We now deduce the consequences of this principle. In applying the power balance (3.4) we are at liberty to choose any $\mathscr{V}$ consistent with the constraint (3.3).

#### 3.2.1. Macroscopic force balances

Consider first a generalized virtual velocity without slip, so that $\tilde{\boldsymbol{\gamma}}\equiv\mathbf{0}$, choose the virtual field $\tilde{\mathbf{u}}$ arbitrarily, and let $\widetilde{\mathbf{E}}^e$ and $\widetilde{\mathbf{W}}^e$ denote the symmetric and skew parts of $\nabla\tilde{\mathbf{u}}$, so that

$$\nabla\tilde{\mathbf{u}} = \widetilde{\mathbf{E}}^e + \widetilde{\mathbf{W}}^e$$

and the constraint (3.3) is satisfied. Then, since $\mathbf{T}$ is symmetric, $\mathbf{T}\cdot\widetilde{\mathbf{E}}^e = \mathbf{T}\cdot\nabla\tilde{\mathbf{u}}$ and the power balance (3.4) takes the form

$$\int_{\partial R}\mathbf{t}(\mathbf{n})\cdot\tilde{\mathbf{u}}\,\mathrm{d}A = \int_R(\mathbf{T}\cdot\nabla\tilde{\mathbf{u}} - \mathbf{f}\cdot\tilde{\mathbf{u}})\,\mathrm{d}V.$$

Equivalently,

$$\int_{\partial R}(\mathbf{t}(\mathbf{n})-\mathbf{T}\mathbf{n})\cdot\tilde{\mathbf{u}}\,\mathrm{d}A=-\int_{R}\tilde{\mathbf{u}}\cdot(\mathrm{div}\,\mathbf{T}+\mathbf{f})\,\mathrm{d}V,$$

and since this relation must hold for all $R$ and all $\tilde{\mathbf{u}}$, a standard argument leads to the traction condition $\mathbf{t}(\mathbf{n})=\mathbf{T}\mathbf{n}$ and the classical local force balance

$$\mathrm{div}\,\mathbf{T}+\mathbf{f}=\mathbf{0}. \tag{3.5}$$

*3.2.2. Microscopic force balances*

To discuss the microscopic counterparts of these results, we define the *resolved shear* $\tau^\alpha$ through

$$\tau^\alpha=\mathbf{s}^\alpha\cdot\mathbf{T}\mathbf{m}^\alpha. \tag{3.6}$$

Consider a generalized virtual velocity with $\tilde{\mathbf{u}}\equiv\mathbf{0}$, choose the virtual field $\tilde{\boldsymbol{\gamma}}$ arbitrarily, and let $\widetilde{\mathbf{E}}^e$ and $\widetilde{\mathbf{W}}^e$ denote the symmetric and skew parts of the tensor field $-\sum_\alpha\tilde{\gamma}^\alpha(\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha)$, so that

$$\sum_{\alpha=1}^{A}\tilde{\gamma}^\alpha(\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha)=-(\widetilde{\mathbf{E}}^e+\widetilde{\mathbf{W}}^e).$$

Then, since $\mathbf{T}$ is symmetric, $\mathbf{T}\cdot\widetilde{\mathbf{E}}^e=-\sum_\alpha\tau^\alpha\tilde{\gamma}^\alpha$ and the power balance (3.4) yields the *microscopic virtual-power relation*

$$\sum_{\alpha=1}^{A}\int_{\partial R}\Xi^\alpha(\mathbf{n})\tilde{\gamma}^\alpha\,\mathrm{d}A=\sum_{\alpha=1}^{A}\int_{R}[(\pi^\alpha-\tau^\alpha)\tilde{\gamma}^\alpha+\boldsymbol{\xi}^\alpha\cdot\nabla\tilde{\gamma}^\alpha]\,\mathrm{d}V \tag{3.7}$$

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

$$\sum_{\alpha=1}^{A}\int_{\partial R}(\Xi^\alpha(\mathbf{n})-\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\tilde{\gamma}^\alpha\,\mathrm{d}A=-\sum_{\alpha=1}^{A}\int_{R}(\mathrm{div}\,\boldsymbol{\xi}^\alpha+\tau^\alpha-\pi^\alpha)\tilde{\gamma}^\alpha\,\mathrm{d}V,$$

and arguing as before this yields the *microtraction conditions*

$$\Xi^\alpha(\mathbf{n})=\boldsymbol{\xi}^\alpha\cdot\mathbf{n} \tag{3.8}$$

and the *microforce balances*

$$\mathrm{div}\,\boldsymbol{\xi}^\alpha+\tau^\alpha-\pi^\alpha=0 \tag{3.9}$$

on each slip system $\alpha$.

## 4. Energy imbalance

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

$$\overline{\int_R\psi\,\mathrm{d}V}^{\cdot}\leqslant\mathscr{P}_{\mathrm{ext}}(R) \tag{4.1}$$

for all subbodies $R$. In view of (3.2) and the identity $\mathscr{P}_{\mathrm{ext}}(R)=\mathscr{P}_{\mathrm{int}}(R)$, (4.1) has the alternative forms

$$\left.\begin{aligned}\overline{\textstyle\int_R\psi\,\mathrm{d}V}^{\cdot}&\leqslant\textstyle\int_{\partial R}\mathbf{T}\mathbf{n}\cdot\dot{\mathbf{u}}\,\mathrm{d}A+\int_R\mathbf{f}\cdot\dot{\mathbf{u}}\,\mathrm{d}V+\sum_{\alpha=1}^{A}\int_{\partial R}(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\dot{\gamma}^\alpha\,\mathrm{d}A,\\ \overline{\textstyle\int_R\psi\,\mathrm{d}V}^{\cdot}&\leqslant\textstyle\int_R\mathbf{T}\cdot\dot{\mathbf{E}}^e\,\mathrm{d}V+\sum_{\alpha=1}^{A}\int_R(\pi^\alpha\dot{\gamma}^\alpha+\boldsymbol{\xi}^\alpha\cdot\nabla\dot{\gamma}^\alpha)\,\mathrm{d}V.\end{aligned}\right\} \tag{4.2}$$

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

$$\dot{\psi} - \mathbf{T} \cdot \dot{\mathbf{E}}^e - \sum_{\alpha=1}^{A} (\boldsymbol{\xi}^\alpha \cdot \nabla \dot{\gamma}^\alpha + \pi^\alpha \dot{\gamma}^\alpha) \leqslant 0. \tag{4.3}$$

We use this 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* $\Psi(\mathbf{G})$:

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

Central to the theory is the thermodynamic *defect stress* defined by

$$\mathbb{T} = \frac{\partial \Psi(\mathbf{G})}{\partial \mathbf{G}}. \tag{5.2}$$

Let $\mathbf{G} = \mathbf{G}(t)$. Then, by (2.2),

$$\overline{\Psi(\mathbf{G})}^{\boldsymbol{\cdot}} = \mathbb{T} \cdot \dot{\mathbf{G}} = \sum_{\alpha=1}^{A} (\nabla \dot{\gamma}^\alpha \times \mathbf{m}^\alpha) \cdot \mathbb{T}\mathbf{s}^\alpha = \sum_{\alpha=1}^{A} (\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) \cdot \nabla \dot{\gamma}^\alpha, \tag{5.3}$$

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 (5.3),

$$\dot{\psi} = \mathbf{C}[\mathbf{E}^e] \cdot \dot{\mathbf{E}}^e + \sum_{\alpha=1}^{A} (\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) \cdot \nabla \dot{\gamma}^\alpha, \tag{5.4}$$

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

$$(\mathbf{T} - \mathbf{C}[\mathbf{E}^e]) \cdot \dot{\mathbf{E}}^e + \sum_{\alpha=1}^{A} [\pi^\alpha \dot{\gamma}^\alpha + (\boldsymbol{\xi}^\alpha - \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) \cdot \nabla \dot{\gamma}^\alpha] \geqslant 0. \tag{5.5}$$

The left side of this inequality represents the *dissipation*, per unit volume. Consider constitutive equations giving $\mathbf{T}$, $\pi^\alpha$, and $\boldsymbol{\xi}^\alpha$ 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 (5.5) hold for all choices of $\dot{\mathbf{E}}^e$, $\dot{\boldsymbol{\gamma}}$, and $\nabla \dot{\boldsymbol{\gamma}}$; the linearity of this inequality in $\dot{\mathbf{E}}^e$ and $\nabla \dot{\boldsymbol{\gamma}}$ then reduces the constitutive equation for $\mathbf{T}$ to the classical form

$$\mathbf{T} = \mathbf{C}[\mathbf{E}^e] \tag{5.6}$$

and—what is more important—requires that

$$\boldsymbol{\xi}^\alpha = \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha. \tag{5.7}$$

Thus (5.5) reduces to $\sum_\alpha \pi^\alpha \dot{\gamma}^\alpha \geqslant 0$. Guided by this inequality and the classical relation (1.5), we posit a constitutive relation for $\pi^\alpha$ in the form

$$\pi^\alpha = \sigma^\alpha f(\dot{\gamma}^\alpha), \tag{5.8}$$

where, for each fixed $\alpha$,

$$f(\dot{\gamma}^\alpha) = -f(-\dot{\gamma}^\alpha), \quad f(\dot{\gamma}^\alpha)\dot{\gamma}^\alpha \geqslant 0, \tag{5.9}$$

and where the *slip resistances* $\sigma^\alpha$ are consistent with the *hardening equations*

$$\dot{\sigma}^\alpha = \sum_{\beta=1}^{A} k^{\alpha\beta}(\sigma^1, \sigma^2, \ldots, \sigma^A)|\dot{\gamma}^\beta|, \qquad \sigma^\alpha(\mathbf{x}, 0) = \sigma_0^\alpha > 0 \tag{5.10}$$

(with hardening moduli $k^{\alpha\beta}$ possibly dependent also on $\mathbf{G}$). The constitutive relations (5.1), (5.7) and (5.8) then satisfy the free-energy inequality. Note that *the microstress* $\boldsymbol{\xi}^\alpha$ *is parallel to the* $\alpha$*th slip plane*, and that $\pi^\alpha$ is dissipative, while $\boldsymbol{\xi}^\alpha$ is energetic.

Note that the constitutive theory is completely specified by the elasticity tensor $\mathbf{C}$, the defect energy $\Psi$, 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 yield conditions

The microforce balance $\operatorname{div}\boldsymbol{\xi}^\alpha + \tau^\alpha - \pi^\alpha = 0$ augmented by the constitutive equations for $\pi^\alpha$ and $\boldsymbol{\xi}^\alpha$ plays the role of a *viscoplastic yield condition*

$$\tau^\alpha - \underbrace{(-1)\operatorname{div}(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha)}_{\text{backstress due to energy stored in dislocations}} = \underbrace{\sigma^\alpha f(\dot{\gamma}^\alpha)}_{\text{dissipative hardening due to slip}} \tag{6.1}$$

for each slip system $\alpha$. 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 $\nabla\nabla\gamma^\beta$, $\beta = 1, 2, \ldots, A$, thereby rendering the yield condition strongly *nonlocal*.

The yield condition (6.1) embodies two different hardening mechanisms: that provided by the hardening equations (5.10) and that which results, via the backstress, from an energetic dependence on $\mathbf{G}$. Hardening imposed by the hardening equation is *strictly dissipative*. This hardening has a purely phenomenological nature; the only restriction placed by the basic theoretical framework is that the slip resistances $\sigma^\alpha$ be nonnegative. Moreover, the resulting hardening *provides no contribution to a backstress*. On the other hand, the hardening resulting from the backstress is *strictly energetic*. This hardening is a consequence of the microforce balance and the restrictions imposed by the thermodynamical framework. [9] It is important to bear in mind that the hardening equations allow for *latent hardening* via the moduli $k^{\alpha\beta}$, $\alpha \neq \beta$. In contrast, hardening arising from the backstress would not directly induce latent hardening; indeed, simple shear is compatible and hence has $\mathbf{G} \equiv \mathbf{0}$, but would generally involve multiple slip and hence latent hardening via (5.10).

Rate-independent yield conditions may be obtained from (6.1) with $f$ of the classical form (1.10) by formally passing to the limit as $\delta \to 0^+$. The result, for each slip system, is as follows (cf. Gurtin, 2000): when the left side of (6.1) lies within the elastic range the slip on $\alpha$ vanishes,

$$-\sigma^\alpha < \tau^\alpha + \operatorname{div}(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) < \sigma^\alpha, \quad \dot{\gamma}^\alpha = 0, \tag{6.2}$$

on the other hand, slip of the right sign is possible when the left side of (6.1) reaches either of the two yield limits,

[9] Cf. the discrete-dislocation computations of Cleveringa et al. (1999), which display large backstresses. These computations are based on plane strain with simple-shear boundary loading, with the specimen a composite consisting of elastic particles within a single-crystal matrix whose only active slip system is parallel to the direction of shear. Computational results of Bittencourt et al. (submitted for publication) comparing the nonlocal theory presented here to the discrete-dislocation theory at micron length scales show qualitative agreement with respect to the backstress. A second set of comparisons, again based on plane strain and simple-shear loading, performed on a pure specimen with two active symmetrically placed slip systems, demonstrate that both hardening mechanisms play essential roles in the emergence of a boundary layer and in the effect of specimen size.

$$\left.\begin{array}{ll}\tau^\alpha + \mathrm{div}(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) = +\sigma^\alpha, & \dot{\gamma}^\alpha \geqslant 0,\\ \tau^\alpha + \mathrm{div}(\mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha) = -\sigma^\alpha, & \dot{\gamma}^\alpha \leqslant 0.\end{array}\right\}. \tag{6.3}$$

For the special case of a *quadratic, isotropic defect energy*

$$\Psi(\mathbf{G}) = \tfrac{1}{2}(c_1|\mathbf{G}|^2 + c_2|\mathrm{tr}\,\mathbf{G}|^2 + c_3|\tfrac{1}{2}(\mathbf{G} - \mathbf{G}^\top)|^2), \tag{6.4}$$

with $c_1$, $c_2$, and $c_3$ constant, the defect stress has the form

$$\mathbb{T} = c_1\mathbf{G} + c_2(\mathrm{tr}\,\mathbf{G})\mathbf{1} + c_3(\mathbf{G} - \mathbf{G}^\top) = (c_1 + c_3)\mathbf{G} + c_2(\mathrm{tr}\,\mathbf{G})\mathbf{1} - c_3\mathbf{G}^\top,$$

or equivalently, by (2.2),

$$\mathbb{T} = \sum_{\beta=1}^{A}((c_1 + c_3)(\nabla\gamma^\beta \times \mathbf{m}^\beta) \otimes \mathbf{s}^\beta + c_2(\nabla\gamma^\beta \cdot \boldsymbol{l}^\beta)\mathbf{1} - c_3\mathbf{s}^\beta \otimes (\nabla\gamma^\beta \times \mathbf{m}^\beta)).$$

Thus, since $\boldsymbol{\xi}^\alpha = \mathbf{m}^\alpha \times \mathbb{T}\mathbf{s}^\alpha$,

$$\boldsymbol{\xi}^\alpha = \sum_{\beta=1}^{A}((c_1 + c_3)(\mathbf{s}^\alpha \cdot \mathbf{s}^\beta)\mathbf{m}^\alpha \times (\nabla\gamma^\beta \times \mathbf{m}^\beta) + c_2(\nabla\gamma^\beta \cdot \boldsymbol{l}^\beta)\boldsymbol{l}^\alpha - c_3(\mathbf{m}^\alpha \times \mathbf{s}^\beta)\nabla\gamma^\beta \cdot (\mathbf{m}^\beta \times \mathbf{s}^\alpha)),$$

and, since $\mathbf{m}^\alpha \times (\nabla\gamma^\beta \times \mathbf{m}^\beta) = [(\mathbf{m}^\alpha \cdot \mathbf{m}^\beta)\mathbf{1} - \mathbf{m}^\beta \otimes \mathbf{m}^\alpha]\nabla\gamma^\beta$, if we define (constant) *tensors*

$$\mathbf{M}^{\alpha\beta} = (c_1 + c_3)(\mathbf{s}^\alpha \cdot \mathbf{s}^\beta)[(\mathbf{m}^\alpha \cdot \mathbf{m}^\beta)\mathbf{1} - \mathbf{m}^\beta \otimes \mathbf{m}^\alpha] + c_2(\boldsymbol{l}^\alpha \otimes \boldsymbol{l}^\beta) - c_3(\mathbf{m}^\alpha \times \mathbf{s}^\beta) \otimes (\mathbf{m}^\beta \times \mathbf{s}^\alpha), \tag{6.5}$$

then the microstress becomes

$$\boldsymbol{\xi}^\alpha = \sum_{\beta=1}^{A}\mathbf{M}^{\alpha\beta}\nabla\gamma^\beta, \tag{6.6}$$

and the yield condition has the explicit form

$$\tau^\alpha + \sum_{\beta=1}^{A}\mathbf{M}^{\alpha\beta} \cdot \nabla\nabla\gamma^\beta = \sigma^\alpha f(\dot{\gamma}^\alpha). \tag{6.7}$$

While the tensors $\mathbf{M}^{\alpha\beta}$ have a complicated form, they are constant and, given the constants $c_1$, $c_2$, and $c_3$, may be computed for any prescribed single crystal. Finally, the *basic equations* of the theory consist of:

(i) the *kinematical equations* (1.1)–(1.4) and (2.2);
(ii) the *macroscopic balance* (3.5) supplemented by the stress–strain relation (5.6);
(iii) the *yield conditions* (6.1) (general theory) or (6.7) (quadratic, isotropic defect energy) supplemented by the hardening equations (5.10).

## 7. The microstress $\xi^\alpha$ as a continuous distribution of Peach–Koehler forces

The present theory is viscoplastic with dislocations distributed continuously throughout the body via a tensor field $\mathbf{G}$. Even so, because there is a natural decomposition of $\mathbf{G}$ into continuous distributions of screw and edge dislocations, one might expect there to be a counterpart of the Peach–Koehler force within the present theory. For a distribution of *pure* dislocations evolving on the $\alpha$th slip plane, such a *distributed* Peach–Koehler force should be parallel to the $\alpha$th slip plane and perpendicular to the line direction; such a force should therefore have the form $\varphi^\alpha_\vdash(\mathbf{m}^\alpha \times \boldsymbol{l}^\alpha)$ for edge dislocations on $\alpha$ and $\varphi^\alpha_\odot(\mathbf{m}^\alpha \times \mathbf{s}^\alpha)$ for screw dislocations on $\alpha$, where the $\varphi$'s are scalar fields that represent associated *force densities*. Further, in the spirit of the classical Peach–Koehler force, these force densities should be energetic in nature. We now give an argument of Gurtin (2002, Section 8.1), showing that if we account for specific dislocations through the decomposition (2.4), then the microstress is a sum of such continuously distributed Peach–Koehler forces. To begin with, note that

$$\overline{\Psi(\mathbf{G})}^{\boldsymbol{\cdot}} = \mathbb{T} \cdot \sum_{\alpha=1}^{A} (\dot{\rho}^{\alpha}_{\odot} \mathbf{s}^{\alpha} \otimes \mathbf{s}^{\alpha} + \dot{\rho}^{\alpha}_{\vdash} \boldsymbol{l}^{\alpha} \otimes \mathbf{s}^{\alpha}) = \sum_{\alpha=1}^{A} (\mathrm{t}^{\alpha}_{\odot} \dot{\rho}^{\alpha}_{\odot} + \mathrm{t}^{\alpha}_{\vdash} \dot{\rho}^{\alpha}_{\vdash}),$$

with

$$\mathrm{t}^{\alpha}_{\odot} = \mathbf{s}^{\alpha} \cdot \mathbb{T}\mathbf{s}^{\alpha}, \qquad \mathrm{t}^{\alpha}_{\vdash} = \boldsymbol{l}^{\alpha} \cdot \mathbb{T}\mathbf{s}^{\alpha}. \tag{7.1}$$

*The fields* $\mathrm{t}^{\alpha}_{\odot}$ *and* $\mathrm{t}^{\alpha}_{\vdash}$ *therefore represent work-conjugate scalar microforces for densities of screw and edge dislocations on the slip system* $\alpha$. These fields therefore represent viable candidates for the force densities associated with such screw and edge dislocations.

Next, fix $\alpha$ and expand $\mathbb{T}$ with respect to the basis $\{\mathbf{s}^{\alpha}, \boldsymbol{l}^{\alpha}, \mathbf{m}^{\alpha}\}$. Then

$$\mathbb{T} = \mathrm{t}^{\alpha}_{\odot} \mathbf{s}^{\alpha} \otimes \mathbf{s}^{\alpha} + \mathrm{t}^{\alpha}_{\vdash} \boldsymbol{l}^{\alpha} \otimes \mathbf{s}^{\alpha} + \mathbb{K},$$

with $\mathbb{K}$ a sum of tensor products of the form $\mathbf{m}^{\alpha} \otimes (\ldots)$, $(\ldots) \otimes \mathbf{m}^{\alpha}$, and $(\ldots) \otimes \boldsymbol{l}^{\alpha}$, so that $\mathbf{m}^{\alpha} \times \mathbb{K}\mathbf{s}^{\alpha} = \mathbf{0}$. Thus, since $\boldsymbol{l}^{\alpha} = \mathbf{m}^{\alpha} \times \mathbf{s}^{\alpha}$, we may use (5.7) to conclude that

$$\boldsymbol{\xi}^{\alpha} = \mathrm{t}^{\alpha}_{\odot}(\mathbf{m}^{\alpha} \times \mathbf{s}^{\alpha}) + \mathrm{t}^{\alpha}_{\vdash}(\mathbf{m}^{\alpha} \times \boldsymbol{l}^{\alpha}). \tag{7.2}$$

Thus the microstress is governed solely by the resolved values $\mathrm{t}^{\alpha}_{\odot}$ and $\mathrm{t}^{\alpha}_{\vdash}$ of the defect stress on the canonical dislocation dyads for $\alpha$. What is more important, the microscopic forces that comprise (7.2) are of the requisite form and hence have the physical interpretations:

$$\underbrace{\mathrm{t}^{\alpha}_{\odot}(\mathbf{m}^{\alpha} \times \mathbf{s}^{\alpha})}_{\text{distributed Peach–Koehler force on screw dislocations}} \qquad \text{and} \qquad \underbrace{\mathrm{t}^{\alpha}_{\vdash}(\mathbf{m}^{\alpha} \times \boldsymbol{l}^{\alpha}).}_{\text{distributed Peach–Koehler force on edge dislocations}}$$

Based on this argument, we view $\boldsymbol{\xi}^{\alpha}$ as a *net distributed Peach–Koehler force* for the slip-system $\alpha$.

Finally, note for future use that (7.2) may be written more simply as

$$\boldsymbol{\xi}^{\alpha} = \mathrm{t}^{\alpha}_{\odot} \boldsymbol{l}^{\alpha} - \mathrm{t}^{\alpha}_{\vdash} \mathbf{s}^{\alpha}.$$

## 8. Microscopically simple boundary conditions

The presence of microstresses results in an expenditure of power $\int_{\partial B} (\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n}) \dot{\gamma}^{\alpha} \, \mathrm{d}A$ by the material in contact with the body, and this necessitates a consideration of boundary conditions on $\partial B$ involving the microtractions $\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n}$ and the slip-rates $\dot{\gamma}^{\alpha}$, where $\mathbf{n}$ denotes the outward unit normal to $\partial B$. We discuss now a simple class of boundary conditions for these fields on a prescribed subsurface $S$ of $\partial B$. These boundary conditions result in a null expenditure of micropower in the sense that $(\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n})\dot{\gamma}^{\alpha} = 0$ on $S$ for all $\alpha$.

The boundary is *microfree* on $S$ if

$$\boldsymbol{\xi}^{\alpha} \cdot \mathbf{n} = 0 \quad \text{on } S, \quad \alpha = 1, 2, \ldots, A. \tag{8.1}$$

This boundary condition would seem consistent with the macroscopic boundary condition $\mathbf{Tn} = \mathbf{0}$ on $S$. By (5.7), $\boldsymbol{\xi}^{\alpha}$ is parallel to the $\alpha$th slip plane, Thus, if the boundary is microfree, then, for each $\alpha$, $\boldsymbol{\xi}^{\alpha}$ (and hence the net Peach–Koehler force on GNDs on $\alpha$) must be tangent to the line of intersection of the $\alpha$th slip plane with $S$. (Other consequences of the microfree conditions are given by Gurtin (2002).)

One might consider the *microclamped* conditions

$$\gamma^{\alpha} = 0 \quad \text{on } S, \quad \alpha = 1, 2, \ldots, A \tag{8.2}$$

in conjunction with a boundary surface $S$ that is macroscopically clamped in the sense that $\mathbf{u} = \mathbf{0}$ on $S$. Consider a microclamped surface. Then, by (8.2), the tangential derivative of $\gamma^\alpha$ must vanish on $S$ for each $\alpha$, so that

$$\nabla\gamma^\alpha = \frac{\partial\gamma^\alpha}{\partial \mathrm{n}}\mathbf{n} \ (\dagger)$$

and, by (2.2),

$$\mathbf{G} = \sum_{\alpha=1}^{A} \frac{\partial\gamma^\alpha}{\partial \mathrm{n}}(\mathbf{n} \times \mathbf{m}^\alpha) \otimes \mathbf{s}^\alpha \quad \text{on } S.$$

$\mathbf{G}$ on $S$ may therefore be considered as the sum over $\alpha$ of mixed dislocations with Burgers direction parallel to $\mathbf{s}^\alpha$ and line direction tangent to the intersection of $S$ with the $\alpha$th slip plane, and with density $|\mathbf{n} \times \mathbf{m}^\alpha|\frac{\partial\gamma^\alpha}{\partial \mathrm{n}}$. Moreover, $\mathbf{G}^\mathsf{T}\mathbf{n} = \mathbf{0}$ on $S$; hence the net Burgers vector associated with small loops on $S$ vanishes. Note also that, by (†),

$$\rho_\vdash^\alpha = -(\mathbf{s}^\alpha \cdot \mathbf{n})\frac{\partial\gamma^\alpha}{\partial \mathrm{n}} \quad \text{and} \quad \rho_\odot^\alpha = (\boldsymbol{l}^\alpha \cdot \mathbf{n})\frac{\partial\gamma^\alpha}{\partial \mathrm{n}} \quad \text{on } S, \tag{8.3}$$

thus

$$\frac{\rho_\odot^\alpha}{\rho_\vdash^\alpha} = -\frac{\boldsymbol{l}^\alpha \cdot \mathbf{n}}{\mathbf{s}^\alpha \cdot \mathbf{n}},$$

which is the assertion that the screw and edge densities for $\alpha$ be in inverse ratio to the projections of their line directions on $\mathbf{n}$. Therefore, $\rho_\odot^\alpha = 0$ or $\mathbf{s}^\alpha \cdot \mathbf{n} = 0$ if and only if $\rho_\vdash^\alpha = 0$ or $\boldsymbol{l}^\alpha \cdot \mathbf{n} = 0$.

## 9. Two-dimensional theory

### 9.1. Strict plane strain

Under plane strain the displacement has the component form

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

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

$$(\nabla\mathbf{u})_{j3} = (\nabla\mathbf{u})_{3j} = 0 \quad (j = 1, 2, 3), \tag{9.1}$$

i.e.,

$$(\nabla\mathbf{u})\mathbf{e} = (\nabla\mathbf{u})^\mathsf{T}\mathbf{e} = \mathbf{0}, \quad \text{with } \mathbf{e} \equiv \mathbf{e}_3, \tag{9.2}$$

the *out-of-plane normal*.

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

$$\mathbf{s}^\alpha \cdot \mathbf{e} = 0, \quad \mathbf{m}^\alpha \cdot \mathbf{e} = 0, \quad \mathbf{s}^\alpha \times \mathbf{m}^\alpha = \mathbf{e}, \tag{9.3}$$

with slips $\gamma^\alpha$ 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 (9.1) and (9.2). There is a large literature based on this *approximative* hypothesis. The resulting fully two-dimensional kinematics, which we refer to as *strict plane strain*, is important in constructing simple mathematical models, often based on two slip systems. [10]

In strict plane strain the lattice rotation $\mathbf{W}^e$ has the form

$$\mathbf{W}^e = \vartheta(\mathbf{e}\times),$$

where $\vartheta(x_1, x_2, t)$, the *lattice-rotation angle*, measures local rotations of the lattice. Then $\mathbf{H}^e = \mathbf{E}^e + \vartheta(\mathbf{e}\times)$ and, since $\mathrm{curl}(\vartheta(\mathbf{e}\times)) = -\mathbf{e} \otimes \nabla\vartheta$, we may use (2.1) to conclude that

$$\mathbf{G} = \mathbf{e} \otimes \nabla\vartheta - \mathrm{curl}\,\mathbf{E}^e. \tag{9.4}$$

### 9.2. Burgers vector g

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

$$\Phi_{,\beta} = \mathbf{s}^\beta \cdot \nabla\Phi, \quad \Phi_{,\alpha\beta} = \mathbf{s}^\alpha \cdot (\nabla\nabla\Phi)\mathbf{s}^\beta, \quad \mathbf{v}_{,\beta} = (\nabla\mathbf{v})\mathbf{s}^\beta. \tag{9.5}$$

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 (2.2),

$$\mathbf{G} = \mathbf{e} \otimes \mathbf{g}, \quad \mathbf{g} = \sum_{\alpha=1}^{A} \gamma^\alpha{}_{,\alpha}\,\mathbf{s}^\alpha. \tag{9.6}$$

Thus, since each slip direction $\mathbf{s}^\alpha$ is orthogonal to $\mathbf{e}$,

$$\mathbf{g} \perp \mathbf{e}.$$

Further, because $\mathbf{g} = \mathbf{G}^{\mathsf{T}}\mathbf{e}$, $\mathbf{g}$ represents the *Burgers vector* (per unit area) for small loops on the cross-sectional plane (the plane with unit normal $\mathbf{e}$). Moreover, (9.6) shows $\mathbf{G}$ to have the form of a single edge dislocation with line direction $\mathbf{e}$ and Burgers vector $\mathbf{g}$.

### 9.3. Constitutive theory—yield conditions

In view of (9.6), we can write the free energy in the form

$$\psi = \tfrac{1}{2}\mathbf{E}^e \cdot \mathbf{C}[\mathbf{E}^e] + \Psi(\mathbf{g}), \tag{9.7}$$

so that, by (9.6),

$$\dot{\psi} = \mathbf{C}[\mathbf{E}^e] \cdot \dot{\mathbf{E}}^e + \sum_{\alpha=1}^{A} (\mathbf{s}^\alpha \cdot \mathbf{t})\dot{\gamma}^\alpha{}_{,\alpha},$$

with

$$\mathbf{t} = \frac{\partial\Psi(\mathbf{g})}{\partial\mathbf{g}}.$$

The free-energy inequality (4.3) therefore takes the form

$$(\mathbf{T} - \mathbf{C}[\mathbf{E}^e]) \cdot \dot{\mathbf{E}}^e + \sum_{\alpha=1}^{A} [\pi^\alpha\dot{\gamma}^\alpha + (\xi^\alpha - (\mathbf{s}^\alpha \cdot \mathbf{t})\mathbf{s}^\alpha) \cdot \nabla\dot{\gamma}^\alpha] \geqslant 0,$$

[10] Cf. e.g., Asaro (1983a,b, pp. 45–46, 84–97 and the references therein).

and arguing as in Section 5, we are led to the relations

$$\boldsymbol{\xi}^\alpha = (\mathbf{s}^\alpha \cdot \mathbf{t})\mathbf{s}^\alpha, \tag{9.8}$$

$\pi^\alpha = f(\dot{\gamma}^\alpha)$, and $\mathbf{T} = \mathbf{C}[\mathbf{E}^e]$. Thus, since $\operatorname{div}\boldsymbol{\xi}^\alpha = \mathbf{s}^\alpha \cdot \nabla(\mathbf{s}^\alpha \cdot \mathbf{t}) = \mathbf{s}^\alpha \cdot \mathbf{t}_{,\alpha}$, the *yield conditions* take the form

$$\tau^\alpha + \mathbf{s}^\alpha \cdot \mathbf{t}_{,\alpha} = \sigma^\alpha f(\dot{\gamma}^\alpha).$$

For the *quadratic, isotropic defect energy*

$$\Psi(\mathbf{g}) = \tfrac{1}{2}c|\mathbf{g}|^2, \tag{9.9}$$

with $c$ constant,

$$\mathbf{t} = c\mathbf{g}$$

and

$$\boldsymbol{\xi}^\alpha = c(\mathbf{s}^\alpha \cdot \mathbf{g})\mathbf{s}^\alpha. \tag{9.10}$$

On the other hand, by (9.6),

$$\mathbf{g} \cdot \mathbf{s}^\alpha = \sum_{\beta=1}^{A} S^{\alpha\beta}\gamma^\beta{}_{,\beta},$$

where $S^{\alpha\beta}$ are the *slip-interaction coefficients*

$$S^{\alpha\beta} = \mathbf{s}^\alpha \cdot \mathbf{s}^\beta.$$

Thus

$$\boldsymbol{\xi}^\alpha = c\left[\sum_{\beta=1}^{A} S^{\alpha\beta}\gamma^\beta{}_{,\beta}\right]\mathbf{s}^\alpha \tag{9.11}$$

and the yield conditions become (cf. $(9.5)_2$)

$$\tau^\alpha + c\sum_{\beta=1}^{A} S^{\alpha\beta}\gamma^\beta{}_{,\beta\alpha} = \sigma^\alpha f(\dot{\gamma}^\alpha). \tag{9.12}$$

By (9.4) and (9.6),

$$\mathbf{g} = \nabla\vartheta - (\operatorname{curl}\mathbf{E}^e)^{\mathsf{T}}\mathbf{e}. \tag{9.13}$$

Thus, when lattice-strain gradients are negligible,

$$\mathbf{g} \approx \nabla\vartheta.$$

Granted this approximation and its second-order counterpart, we have the following approximate forms for the microstresses and yield conditions:

$$\boldsymbol{\xi}^\alpha \approx c\vartheta_{,\alpha}\mathbf{s}^\alpha, \qquad \tau^\alpha + c\vartheta_{,\alpha\alpha} \approx \sigma^\alpha f(\dot{\gamma}^\alpha).$$

In this approximation, $\boldsymbol{\xi}^\alpha$ is linear in $\vartheta_{,\alpha}$, which is the curvature of the deformed $\alpha$th slip line, [11] and the nonlocal term $\vartheta_{,\alpha\alpha}$ in the yield condition, which characterizes the backstress, represents the change of this curvature in the direction of slip on $\alpha$.

[11] At least to within the approximations inherent in the underlying hypothesis of small deformations.

## 10. Grain boundaries

In this section we develop kinematical and mechanical transmission conditions across a boundary between crystalline grains.

### 10.1. Kinematics

We assume that the bulk material within each grain is consistent with the theory developed in the preceding sections. We write $\mathbf{R}$ (defined uniquely up to a symmetry transformation of the crystal) for the prescribed orthogonal tensor that defines the relative misorientation of grain 2 relative to grain 1, before deformation. We assume that the slip systems of the individual grains are labelled in a manner consistent with this misorientation, so that, labelling the grains $i = 1, 2$ and writing $\mathbf{s}_i^\alpha$ and $\mathbf{m}_i^\alpha$ for the slip directions and slip-plane normals for grain $i$,

$$\mathbf{s}_2^\alpha = \mathbf{R}\mathbf{s}_1^\alpha \quad \text{and} \quad \mathbf{m}_2^\alpha = \mathbf{R}\mathbf{m}_1^\alpha \tag{10.1}$$

for each slip system $\alpha$.

Let $S$ denote the smooth surface that represents the grain boundary, and let $\mathbf{n}_S$ denote the the unit normal to $S$, directed outward from grain 1. We assume that the bulk fields are smooth away from $S$ and up to $S$ from each grain; given any bulk field $\varphi$, we write $\varphi_1$ for the limit of $\varphi$ at $S$ from grain 1, $\varphi_2$ for the limit of $\varphi$ from grain 2, and $[\![\varphi]\!] = \varphi_2 - \varphi_1$ for the *jump* of $\varphi$ across $S$. Then, by (1.4) and (10.1),

$$[\![\mathbf{H}^p]\!] = \sum_{\alpha=1}^{A} [\![\gamma^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha]\!] = \sum_{\alpha=1}^{A} \gamma_2^\alpha \mathbf{s}_2^\alpha \otimes \mathbf{m}_2^\alpha - \sum_{\alpha=1}^{A} \gamma_1^\alpha \mathbf{s}_1^\alpha \otimes \mathbf{m}_1^\alpha. \tag{10.2}$$

To exclude cavitation at the grain boundary we require that the normal component of the displacement $\mathbf{u}$ be continuous across $S$:

$$[\![\mathbf{u}]\!] \cdot \mathbf{n}_S = 0. \tag{10.3}$$

The jump $[\![\mathbf{u}]\!]$, which is tangential to $S$, represents *grain-boundary slip*.

### 10.2. Force balances at the grain boundary

Let $R$ be an arbitrary subregion of the body and assume that

$$S_R = S \cap R,$$

the portion $S_R$ of $S$ in $R$, is a smooth subsurface. Let $\varphi$ denote a bulk field, so that $\varphi$ may suffer a jump discontinuity across $S$. Then integrals such as $\int_R \nabla\varphi \, \mathrm{d}V$, $\int_R \dot{\varphi} \, \mathrm{d}V$, and $\int_{\partial R} \dot{\varphi} \, \mathrm{d}A$ are treated as ordinary integrals with piecewise continuous integrands; e.g., the first integral is given as the integrals of $\nabla\varphi$ over the portion of $R$ in grain 1 plus the integral over the portion of $R$ in grain 2.

We neglect surface stresses within $S$ that act on $S_R$ along its boundary curve $\partial S_R$. The external power expenditure for $R$ is thus, as before, given by $(3.2)_1$, so that, since $\mathbf{t}(\mathbf{n}) = \mathbf{T}\mathbf{n}$,

$$\mathscr{P}_{\mathrm{ext}}(R) = \int_{\partial R} \mathbf{T}\mathbf{n} \cdot \dot{\mathbf{u}} \, \mathrm{d}A + \int_R \mathbf{f} \cdot \dot{\mathbf{u}} \, \mathrm{d}V + \sum_{\alpha=1}^{A} \int_{\partial R} (\boldsymbol{\xi}^\alpha \cdot \mathbf{n}) \dot{\gamma}^\alpha \, \mathrm{d}A. \tag{10.4}$$

The internal power consists of the bulk portion $(3.2)_2$ augmented by the contribution due to the presence of the grain boundary. The basic kinematic quantities that act internally to $S_R$ are the slip-velocity $[\![\dot{\mathbf{u}}]\!]$ and the limiting slip rates $\dot{\gamma}_1^\alpha$ and $\dot{\gamma}_2^\alpha$; to accomodate these we introduce a macroscopic internal force $\boldsymbol{\tau}$ conjugate to $[\![\dot{\mathbf{u}}]\!]$ and microscopic internal forces $\Pi_1^\alpha$ and $\Pi_2^\alpha$ conjugate to $\dot{\gamma}_1^\alpha$ and $\dot{\gamma}_2^\alpha$. We therefore write the internal power in the form

$$\mathscr{P}_{\rm int}(R) = \int_R \mathbf{T}\cdot\dot{\mathbf{E}}^e\,{\rm d}V + \sum_{\alpha=1}^{A}\int_R (\pi^\alpha\dot{\gamma}^\alpha + \boldsymbol{\xi}^\alpha\cdot\nabla\dot{\gamma}^\alpha)\,{\rm d}V + \int_{S_R}\boldsymbol{\tau}\cdot[\![\dot{\mathbf{u}}]\!]\,{\rm d}A + \sum_{\alpha=1}^{A}\int_{S_R}(\Pi_1^\alpha\dot{\gamma}_1^\alpha + \Pi_2^\alpha\dot{\gamma}_2^\alpha)\,{\rm d}A. \tag{10.5}$$

Consistent with the constraint $\mathbf{n}_S\cdot[\![\dot{\mathbf{u}}]\!] = 0$, we require that $\boldsymbol{\tau}$ be tangential:

$$\boldsymbol{\tau}\cdot\mathbf{n}_S = 0.$$

We define virtual velocities as in Section 3.1, except we now add the grain-boundary constraint $\mathbf{n}_S\cdot[\![\tilde{\mathbf{u}}]\!] = 0$. Then, as before, the *principle of virtual power* requires that $\mathscr{P}_{\rm ext}(R,\mathscr{V}) = \mathscr{P}_{\rm int}(R,\mathscr{V})$ for all $R$ and all virtual velocity fields $\mathscr{V}$. We decouple the grain boundary from the bulk material by choosing an arbitrary subsurface $P$ of $S$ and a subregion $R$ such that $S_R = P$, and then shrinking R smoothly down to $P$. In this process the limiting values of the integrals over $R$ vanish, since the volume of $R$ vanishes, while

$$\int_{\partial R}\mathbf{T}\mathbf{n}\cdot\tilde{\mathbf{u}}\,{\rm d}A \to \int_P [\![\mathbf{T}\mathbf{n}_S\cdot\tilde{\mathbf{u}}]\!]\,{\rm d}A, \qquad \int_{\partial R}(\boldsymbol{\xi}^\alpha\cdot\mathbf{n})\tilde{\gamma}^\alpha\,{\rm d}A \to \int_P [\![(\boldsymbol{\xi}^\alpha\cdot\mathbf{n}_S)\tilde{\gamma}^\alpha]\!]\,{\rm d}A;$$

and we are therefore led to a virtual power principle for a "pillbox" $P$ of infinitesimal thickness:

$$\int_P [\![\mathbf{T}\mathbf{n}_S\cdot\tilde{\mathbf{u}}]\!]\,{\rm d}A + \sum_{\alpha=1}^{A}\int_P [\![(\boldsymbol{\xi}^\alpha\cdot\mathbf{n}_S)\tilde{\gamma}^\alpha]\!]\,{\rm d}A = \int_P \boldsymbol{\tau}\cdot[\![\tilde{\mathbf{u}}]\!]\,{\rm d}A + \sum_{\alpha=1}^{A}\int_P(\Pi_1^\alpha\tilde{\gamma}_1^\alpha + \Pi_2^\alpha\tilde{\gamma}_2^\alpha)\,{\rm d}A; \tag{10.6}$$

since $P$ is arbitrary,

$$[\![\mathbf{T}\mathbf{n}_S\cdot\tilde{\mathbf{u}}]\!] + \sum_{\alpha=1}^{A}[\![(\boldsymbol{\xi}^\alpha\cdot\mathbf{n}_S)\tilde{\gamma}^\alpha]\!] = \boldsymbol{\tau}\cdot[\![\tilde{\mathbf{u}}]\!] + \sum_{\alpha=1}^{A}(\Pi_1^\alpha\tilde{\gamma}_1^\alpha + \Pi_2^\alpha\tilde{\gamma}_2^\alpha), \tag{10.7}$$

a relation that must hold for all fields $\tilde{\gamma}_1^\alpha$, $\tilde{\gamma}_2^\alpha$, $\tilde{\mathbf{u}}_1$, and $\tilde{\mathbf{u}}_2$ on $S$ consistent with the constraint $\tilde{\mathbf{u}}_1\cdot\mathbf{n}_S = \tilde{\mathbf{u}}_2\cdot\mathbf{n}_S$. Assume first that the $\tilde{\gamma}^\alpha$'s vanish identically. The choice $\tilde{\mathbf{u}}_1 = \tilde{\mathbf{u}}_2$ then yields the classical balance

$$[\![\mathbf{T}]\!]\mathbf{n}_S = \mathbf{0}, \tag{10.8}$$

and we may use the abbreviation

$$\mathbf{T}\mathbf{n}_S = \mathbf{T}_1\mathbf{n}_S = \mathbf{T}_2\mathbf{n}_S. \tag{10.9}$$

On the other hand, the choice $\tilde{\mathbf{u}}_1 = \mathbf{0}$ yields $(\mathbf{T}\mathbf{n}_S - \boldsymbol{\tau})\cdot\tilde{\mathbf{u}}_2 = 0$ for all $\tilde{\mathbf{u}}_2$ tangent to $S$; since $\boldsymbol{\tau}$ is tangential, this implies that $(\mathbf{T}\mathbf{n}_S)_{\rm tan} = \boldsymbol{\tau}$. (Here $\mathbf{a}_{\rm tan}$ denotes the tangential component of a vector $\mathbf{a}$; i.e., $\mathbf{a}_{\rm tan} = \mathbf{a} - (\mathbf{a}\cdot\mathbf{n}_S)\mathbf{n}_S$.) Thus and by (10.8),

$$(\mathbf{T}\mathbf{n}_S)_{\rm tan} = \boldsymbol{\tau}. \tag{10.10}$$

Finally, if we choose $\tilde{\mathbf{u}} \equiv \mathbf{0}$ in (10.7) and use the fact that for each $\alpha$, $\tilde{\gamma}_1^\alpha$ and $\tilde{\gamma}_2^\alpha$ are each arbitrary, we are led to microforce balances for the grain boundary: for each slip system $\alpha$,

$$\boldsymbol{\xi}_1^\alpha\cdot\mathbf{n}_S = -\Pi_1^\alpha, \qquad \boldsymbol{\xi}_2^\alpha\cdot\mathbf{n}_S = \Pi_2^\alpha. \tag{10.11}$$

### *10.3. Energy imbalance*

Neglecting grain-boundary energy, the inequality (4.1) remains the appropriate form of the second law in all motions of the body. Moreover, since $S$ is time-independent,

$$\overline{\int_R \psi \, dV}^{\cdot} = \int_R \dot{\psi} \, dV. \tag{10.12}$$

As before, we shrink $R$ to an arbitrary subsurface $P$ of $S$. Then (10.12) vanishes and, since $\mathscr{P}_{\text{ext}}(R) = \mathscr{P}_{\text{int}}(R)$ with $\mathscr{P}_{\text{int}}(R)$ given by (10.5), and since $P$ is arbitrary, we are led to the *dissipation inequality*

$$\boldsymbol{\tau} \cdot [\![\dot{\mathbf{u}}]\!] + \sum_{\alpha=1}^{A} (\Pi_1^\alpha \dot{\gamma}_1^\alpha + \Pi_2^\alpha \dot{\gamma}_2^\alpha) \geqslant 0. \tag{10.13}$$

We close the theory by specifying constitutive equations for the internal microforces $\Pi_1^\alpha$ and $\Pi_2^\alpha$ and the grain-boundary shear stress $\boldsymbol{\tau}$.

### 10.4. Constitutive relations

With a view toward specifying orientational variables appropriate to constitutive equations for the grain boundary, consider a fixed reference lattice and let $\mathbf{R}_1$ and $\mathbf{R}_2$ denote the orthogonal tensors that define the relative orientations of grains 1 and 2 relative to this fixed lattice. Further, let $\bar{\mathbf{s}}^\alpha$ and $\bar{\mathbf{m}}^\alpha$ denote the slip direction and slip plane normal for $\alpha$ measured in the reference lattice and define the slip-orientation pair $O_1^\alpha$ by

$$O_1^\alpha = (|\mathbf{R}_1^\top \mathbf{n}_S \cdot \bar{\mathbf{s}}^\alpha|, |\mathbf{R}_1^\top \mathbf{n}_S \cdot \bar{\mathbf{m}}^\alpha|). \tag{10.14}$$

Appropriate variables for grain 1 would then seem to be the normal $\mathbf{R}_1^\top \mathbf{n}_S$ to the grain-boundary *in the reference lattice* measured with respect to grain 1, the misorientation $\mathbf{R}_2\mathbf{R}_1^\top$ relative to grain 1, and the slip-orientation pair $O_1^\alpha$:

$$(\mathbf{R}_2\mathbf{R}_1^\top, \mathbf{R}_1^\top \mathbf{n}_S, O_1^\alpha).$$

Similarly, reversing the roles of the two grains in (10.14), the appropriate variables for grain 2 would be

$$(\mathbf{R}_1\mathbf{R}_2^\top, \mathbf{R}_2^\top \mathbf{n}_S, O_2^\alpha),$$

with $O_2^\alpha$ the natural counterpart of (10.14) for grain 2. If we identify the reference lattice with the lattice as oriented in grain 1, then $\mathbf{R}_1 = \mathbf{1}$, $\mathbf{R} = \mathbf{R}_2$, $\mathbf{s}_1^\alpha = \bar{\mathbf{s}}^\alpha$, $\mathbf{m}_1^\alpha = \bar{\mathbf{m}}^\alpha$, $\mathbf{s}_2^\alpha = \mathbf{R}\bar{\mathbf{s}}^\alpha$, $\mathbf{m}_2^\alpha = \mathbf{R}\bar{\mathbf{m}}^\alpha$,

$$O_1^\alpha = (|\mathbf{n}_S \cdot \mathbf{s}_1^\alpha|, |\mathbf{n}_S \cdot \mathbf{m}_1^\alpha|), \qquad O_2^\alpha = (|\mathbf{n}_S \cdot \mathbf{s}_2^\alpha|, |\mathbf{n}_S \cdot \mathbf{m}_2^\alpha|),$$

and the appropriate orientational variables for grains 1 and 2, respectively, become

$$(\mathbf{R}, \mathbf{n}_S, O_1^\alpha) \quad \text{and} \quad (\mathbf{R}^\top, \mathbf{R}^\top \mathbf{n}_S, O_2^\alpha).$$

Guided by the foregoing discussion, the bulk constitutive equations (5.8), and the dissipation inequality (10.13), we assume that there is a constitutive function $\Phi > 0$ and a scalar $\delta > 0$ such that

$$\left.\begin{aligned} \Pi_1^\alpha &= \zeta_1^\alpha |\dot{\gamma}_1^\alpha|^\delta \operatorname{sgn} \dot{\gamma}_1^\alpha, \qquad & \zeta_1^\alpha &= \kappa \Phi(\mathbf{R}, \mathbf{n}_S, O_1^\alpha), \\ \Pi_2^\alpha &= \zeta_2^\alpha |\dot{\gamma}_2^\alpha|^\delta \operatorname{sgn} \dot{\gamma}_2^\alpha, \qquad & \zeta_2^\alpha &= \kappa \Phi(\mathbf{R}^\top, \mathbf{R}^\top \mathbf{n}_S, O_2^\alpha), \end{aligned}\right\} \tag{10.15}$$

where $\kappa > 0$, defined by

$$\dot{\kappa} = -h(\kappa) \sum_{\beta=1}^{A} (|\dot{\gamma}_1^\beta| + |\dot{\gamma}_2^\beta|), \quad \kappa(\mathbf{x}, 0) = 1 \tag{10.16}$$

represents softening (or hardening) due to slip accumulated at the grain boundary. (We would expect softening, since the continued accumulation of slip should induce disorder in the grain boundary.)

We assume that the shear stress $\boldsymbol{\tau}$ is a function of the grain-boundary slip-rate

$$\mathbf{d} = [\![\dot{\mathbf{u}}]\!].$$

We consider a simple constitutive relation for $\boldsymbol{\tau}$ of a form similar to that assumed for $\Pi_i^\alpha$, in which the role of $\operatorname{sgn}\dot{\gamma}_1^\alpha$ is replaced by the grain-boundary slip-direction $\mathbf{d}/|\mathbf{d}|$. Precisely, we assume that

$$\boldsymbol{\tau} = \kappa\varphi(\mathbf{n}_S, \mathbf{R})|\mathbf{d}|^\delta \frac{\mathbf{d}}{|\mathbf{d}|}, \tag{10.17}$$

with $\varphi > 0$, so that, by (10.16), the accumulation of bulk slip at the grain boundary induces softening in the relation between $\boldsymbol{\tau}$ and $\mathbf{d}$.

It is clear that the constitutive relations developed above are consistent with the dissipation inequality (10.13).

### *10.5. Viscoplastic yield conditions for the grain-boundary*

The force balances (10.10) and (10.11) supplemented by the constitutive relations (10.15) and (10.17) play the role of viscoplastic yield conditions for the grain boundary. These consist of the *microtraction conditions*

$$\left.\begin{aligned} -\boldsymbol{\xi}_1^\alpha \cdot \mathbf{n}_S &= \zeta_1^\alpha|\dot{\gamma}_1^\alpha|^\delta \operatorname{sgn}\dot{\gamma}_1^\alpha, \quad \zeta_1^\alpha = \kappa\Phi(\mathbf{R}, \mathbf{n}_S, O_1^\alpha), \\ \boldsymbol{\xi}_2^\alpha \cdot \mathbf{n}_S &= \zeta_2^\alpha|\dot{\gamma}_2^\alpha|^\delta \operatorname{sgn}\dot{\gamma}_2^\alpha, \quad \zeta_2^\alpha = \kappa\Phi(\mathbf{R}^\top, \mathbf{R}^\top\mathbf{n}_S, O_2^\alpha,) \end{aligned}\right\} \tag{10.18}$$

for each slip system $\alpha$, where $\kappa$ satisfies (10.16), together with a condition

$$(\mathbf{T}\mathbf{n}_S)_{\tan} = \kappa\varphi(\mathbf{n}_S, \mathbf{R})|\mathbf{d}|^\delta \frac{\mathbf{d}}{|\mathbf{d}|} \tag{10.19}$$

for the *macroscopic shear stress*.

Note that $\Phi(\mathbf{R}, \mathbf{n}_S, O_1^\alpha)$, $\Phi(\mathbf{R}^\top, \mathbf{R}^\top\mathbf{n}_S, O_2^\alpha)$, and $\varphi(\mathbf{n}_S, \mathbf{R})$ are prescribed once and for all, given the misorientation, the grain-boundary normal, and the Schmid tensors for the individual slip systems. Moreover, these moduli are independent of time and dependent on $\mathbf{x}$ only when the grain boundary is nonplanar.

In most cases of interest the rate dependence is small. In fact, the rate-independent theory offers insight into the implications of the grain boundary conditions. The rate independent limit of (10.18) is obtained by formally passing to the limit as $\delta \to 0^+$. The result for grain $i$ and slip system $\alpha$ may be stated as follows: when the microtraction lies within the yield range the slip on $\alpha$ at the grain-boundary vanishes,

$$-\zeta_i^\alpha < (-1)^i\boldsymbol{\xi}_i^\alpha \cdot \mathbf{n}_S < \zeta_i^\alpha, \quad \dot{\gamma}_i^\alpha = 0, \tag{10.20}$$

on the other hand, when the microtraction reaches either of the two yield limits, then slip of the right sign is possible,

$$\left.\begin{aligned} (-1)^i\boldsymbol{\xi}_i^\alpha \cdot \mathbf{n}_S &= +\zeta_i^\alpha, \quad \dot{\gamma}_i^\alpha \geqslant 0, \\ (-1)^i\boldsymbol{\xi}_i^\alpha \cdot \mathbf{n}_S &= -\zeta_i^\alpha, \quad \dot{\gamma}_i^\alpha \leqslant 0. \end{aligned}\right\} \tag{10.21}$$

Thus, in contrast to the bulk yield conditions (6.2) and (6.3), the condition (10.20) and (10.21) mark a transition in boundary conditions from the kinematic condition $\dot{\gamma}_i^\alpha = 0$ (cf. (8.2)) to a microtraction condition prescribing $\boldsymbol{\xi}_i^\alpha \cdot \mathbf{n}_S$. Further, grain boundary flow requires a content of GNDs sufficient to drive the microtraction to its yield value, and for that reason would generally occur sometime after yield has occured within the adjacent bulk material. The rate-independent limit of (10.19) has a strictly analogous form and marks a change in boundary condition from null macroscopic slip to a condition on the common value of the macroscopic shear stress.

## 11. Strict plane strain

### 11.1. General remarks

Next, by (9.10), the microstress conditions (10.18) at the grain boundary take the form

$$c(\mathbf{s}_1^\alpha \cdot \mathbf{g})\mathbf{s}_1^\alpha \cdot \mathbf{n}_S = -\zeta_1^\alpha |\dot{\gamma}_1^\alpha|^\delta \operatorname{sgn} \dot{\gamma}_1^\alpha, \qquad c(\mathbf{s}_2^\alpha \cdot \mathbf{g})\mathbf{s}_2^\alpha \cdot \mathbf{n}_S = \zeta_2^\alpha |\dot{\gamma}_2^\alpha|^\delta \operatorname{sgn} \dot{\gamma}_2^\alpha, \tag{11.1}$$

$\alpha = 1, \ldots, A$, relations that may also be written in terms of the slip gradients using (9.11). The result (11.1) has an interesting consequence that is most easily discussed within a *rate independent* setting ($\delta = 0$). The grain-boundary conditions then require that for, say slip system $\alpha$ in grain 1, $-c(\mathbf{s}_1^\alpha \cdot \mathbf{g})\mathbf{s}_1^\alpha \cdot \mathbf{n}_S$ lie between $\pm\zeta_1^\alpha$, with flow possible at the grain boundary on $\alpha$ only when one of the values $\pm\zeta_1^\alpha$ is attained. Thus (11.1) implies that

$$\mathbf{s}_i^\alpha \cdot \mathbf{g}_i = \bar{\zeta}_i^\alpha, \quad \bar{\zeta}_i^\alpha = (-1)^i \frac{\zeta_i^\alpha \operatorname{sgn} \dot{\gamma}_i^\alpha}{c(\mathbf{s}_i^\alpha \cdot \mathbf{n}_S)}$$

for each grain $i$ and each *active* slip system $\alpha$ for grain $i$ that is *nontangent* in the sense that $\mathbf{s}_i^\alpha \cdot \mathbf{n}_S \neq 0$. Then, neglecting softening as described by (10.16), $\bar{\zeta}_i^\alpha$ is independent of time and, if the interface is planar, also independent of $\mathbf{x}$. In any event, if there are at least two active nontangent slip systems for grain $i$, then $\mathbf{g}_i$ *is temporally constant:*

$$\dot{\mathbf{g}}_i = \mathbf{0}. \tag{11.2}$$

The foregoing conditions have interesting and important consequences. Consider a body under monotone increasing loading, and neglect grain boundary softening or hardening ($\kappa \equiv 1$).

(a) In the initial stages following the onset of plastic flow, the Burgers vector $\mathbf{g}$ in each grain should be small and hence the microtraction conditions (10.20) would imply that $\dot{\gamma}_i^\alpha = 0$ for both grains and all slip systems. Thus in this initial stage the grain boundary acts as a *barrier* for plastic slip. Moreover, the constraints $\dot{\gamma}_i^\alpha = 0$ should induce increasing slip gradients on each of the slip systems near $S$ and this in turn should result in an increase in the magnitude of $\mathbf{g}$ at $S$ in each of the grains. This effect should be local and not apparent away from the grain boundary, where the accumulation of GNDs would be of lesser magnitude. Thus we would expect $|\mathbf{g}|$ to exhibit a sharp peak during the initial stages of the loading.

(b) As the loading increases the Burgers vector $\mathbf{g}$ should increase in magnitude until for some grain $i$ and nontangent slip system $\alpha$, $\mathbf{s}_i^\alpha \cdot \mathbf{g}_i$ reaches the threshold value $\bar{\zeta}_i^\alpha$. At this point, although the loading continues to increase, $\mathbf{s}_i^\alpha \cdot \mathbf{g}_i$ can no longer increase. Further, if on a second nontangent slip system $\beta$ in grain $i$, $\mathbf{s}_i^\beta \cdot \mathbf{g}_i$ reaches its threshold value, and if both $\mathbf{s}_i^\alpha \cdot \mathbf{g}_i$ and $\mathbf{s}_i^\beta \cdot \mathbf{g}_i$ remain at their threshold values, as would be expected, then $\mathbf{g}_i$ itself cannot thereafter vary with time.

The behavior specified in (a) and (b), which is a consequence of the microtraction conditions at the grain boundary seems consistent with the experiments of Sun et al. (1998, 2000).

Finally, if the material is mildly rate dependent, then one would expect the behaviour described in (a) and (b), at least qualitatively.

### 11.2. An explicit solution: accumulation of GNDs at the grain boundary

We now describe an example, within the context of strict plane strain, for which an explicit analytical solution can be found. As we shall see, the qualitative behavior of this solution is consistent with the discussion in (a) and (b) above.

This solution involves a semi-infinite compressed specimen that abuts a rigid material and has two active slip systems symmetrically oriented with respect to the axis of compression. The solution, which is exact,

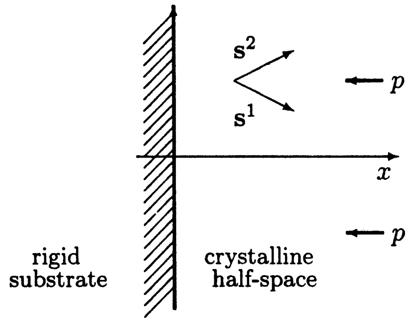


Fig. 1. Simplified model of a grain boundary between a grain with slip systems aligned for easy flow and a grain whose slip system alignment severely inhibits flow.

may be viewed as an approximation to a situation involving a grain boundary between a grain with slip systems aligned for easy flow and a grain whose slip system alignment severely inhibits flow (Fig. 1).

Precisely, we consider a single-crystal occupying the half-plane $\{(x_1,x_2) : x_1 > 0\}$, with grain boundary the line $x_1 = 0$. Since the adjacent crystal, say crystal 2, is viewed as rigid, we may restrict attention to grain 1 and, without danger of confusion, omit the subscript 1 when it labels that grain. We assume that only two slip systems are active and that the $x_1$-axis is an axis of symmetry of the crystal; we therefore let

$$\begin{aligned} \mathbf{s}^1 &= \cos\tfrac{\theta}{2}\mathbf{e}_1 - \sin\tfrac{\theta}{2}\mathbf{e}_2, \qquad & \mathbf{m}^1 &= \sin\tfrac{\theta}{2}\mathbf{e}_1 + \cos\tfrac{\theta}{2}\mathbf{e}_2, \\ \mathbf{s}^2 &= \cos\tfrac{\theta}{2}\mathbf{e}_1 + \sin\tfrac{\theta}{2}\mathbf{e}_2, \qquad & \mathbf{m}^2 &= -\sin\tfrac{\theta}{2}\mathbf{e}_1 + \cos\tfrac{\theta}{2}\mathbf{e}_2, \end{aligned} \tag{11.3}$$

with $\theta$ a fixed angle and $\mathbf{e}_1$ and $\mathbf{e}_2$ the unit vectors that mark the $x_1$ and $x_2$ axes.

We restrict attention to a simplified situation in which all fields are independent of $x_2$, and write $x$ for $x_1$. The basic unknowns of the problem are the displacement $\mathbf{u}$ and the slips $\gamma^\alpha$, and we assume that the displacement is horizontal and the slip is symmetric with respect to the $x$-axis, i.e.,

$$\mathbf{u} = u\mathbf{e}_1, \qquad \gamma^1 = -\gamma^2 =: \gamma. \tag{11.4}$$

For simplicity, we restrict attention to the rate-independent theory, but allow for bulk hardening and grain-boundary softening. We assume that the bulk hardening matrix $k^{\alpha\beta}$ in (5.10) is constant and symmetric with $k^{11} = k^{22}$. Thus $\sigma^1 = \sigma^2 =: \sigma$ satisfies

$$\dot{\sigma} = k|\dot{\gamma}|, \qquad \sigma(x,0) = \sigma_0 > 0, \tag{11.5}$$

with $k = k^{11} + k^{12} = k^{12} + k^{22} > 0$.

By symmetry and since the grain boundary is flat, $\Phi(\mathbf{R}, \mathbf{n}_S, O_1^\alpha)$ is constant and independent of $\alpha$. We assume that the function $h$ that characterizes grain-boundary softening is strictly positive and constant. Thus, by (10.15) and (10.16), the slip resistances $\zeta_1 = \zeta_2 =: \zeta$ for the grain boundary evolve according to

$$\dot{\zeta} = \begin{cases} -h|\dot{\gamma}|, & \bar{\zeta}_0 < \zeta < \zeta_0 = \zeta(0), \\ 0, & \zeta = \bar{\zeta}_0, \end{cases} \tag{11.6}$$

with $\zeta_0 = \Phi$, $\bar{\zeta}_0$ and $h$ positive constants. The truncation of (11.6) at $\bar{\zeta}_0$ means that the grain boundary cannot soften indefinitely.

We look for solutions of the equilibrium equation $\operatorname{div}\mathbf{T} = \mathbf{0}$ (cf. (3.5)) supplemented by the rate-independent yield conditions (6.2) and (6.3). Regarding the boundary conditions, we assume that a compressive load is applied at $x = \infty$, i.e.,

$$\mathbf{T}\mathbf{e}_1 \to -p\mathbf{e}_1 \quad \text{as } x \to \infty, \tag{11.7}$$

where the loading $p = p(t) > 0$ is a *positive, monotone increasing function of time*. In conjunction with this we assume that no microtraction acts on the crystal at infinity,

$$\boldsymbol{\xi}^{\alpha} \cdot \mathbf{e}_1 \to 0 \quad \text{as } x \to \infty. \tag{11.8}$$

At the grain boundary $x = 0$, we have the condition

$$\mathbf{u}(0, t) = \mathbf{0} \tag{11.9}$$

as well as the rate-independent grain-boundary yield conditions (10.20) and (10.21).

In this simple setting, the displacement $u$ and the slip $\gamma$ may be determined explicitly as functions of $(x, t)$. Since $p(t)$ is invertible with respect to time, we shall write $u$ and $\gamma$ as functions of $x$ and the loading $p$. [12]

We prefer to state the solution first and then give its derivation. Letting $E$ denote Young's modulus and $v$ Poisson's ratio, and recalling that $c$ and $k$ are defined in (9.9) and (11.5), the parameters and functions involved in the solution consist of:

(a) a *boundary layer thickness*

$$L = \sqrt{\frac{c(1 - v^2)\sin^2\theta}{E\sin^2\theta + 2k(1 - v^2)}} > 0; \tag{11.10}$$

(b) *pressures*

$$p_1 = \frac{2(1 - v)}{(1 - 2v)\sin\theta}\sigma_0, \quad p_2 = \frac{2(1 - v)}{(1 - 2v)\sin\theta}\left(\sigma_0 + \frac{\zeta_0}{L}\right), \quad \text{and}$$

$$p_3 = \frac{2(1 - v)}{(1 - 2v)\sin\theta}\left[\sigma_0 + \frac{\zeta_0}{L} + \frac{\zeta_0 - \bar{\zeta}_0}{L}\left(\frac{c\sin^2\theta}{2hL} - 1\right)\right]; \tag{11.11}$$

(c) *bulk and grain boundary forcing functions*

$$r(p) = \frac{L^2(1 - 2v)}{c(1 - v)\sin\theta}(p - p_1) \quad \text{and} \quad s(p) = \frac{2L(\zeta_0 - hr(p))}{c\sin^2\theta - 2hL}. \tag{11.12}$$

(Note that $s(p_2) = r(p_2)$ and that $r(p)$ is an increasing function of the loading, while $s(p)$ is decreasing.)

Our solution may then be stated as follows:

(i) For $p < p_1$, the material behaves elastically, i.e., $\gamma(x, p) \equiv 0$.

(ii) For $p_1 \leqslant p < p_2$,

$$\gamma(x, p) = -r(p)(1 - \mathrm{e}^{-x/L}), \tag{11.13}$$

where $r(p)$, given by $(11.12)_1$, is a linear increasing function of $p$. In this loading range, $\gamma(0, p) = 0$ and the grain boundary is microclamped: $p_2$ is in fact the threshold for the activation of slip at the grain boundary. Moreover, the GND edge densities for the two available slip systems coincide, and writing

$$\rho_{\vdash} := \rho^1_{\vdash} = \rho^2_{\vdash},$$

we have

$$\rho_{\vdash}(x, p) = \frac{r(p)\sin\theta}{L}\mathrm{e}^{-x/L} \tag{11.14}$$

[12] Rather than of $x$ and $t$. By rate independence, time only occurs as a parameter in the equations for $u$ and $\gamma$, so that it is meaningful to choose the loading as the parameter controlling the evolution of the solution.

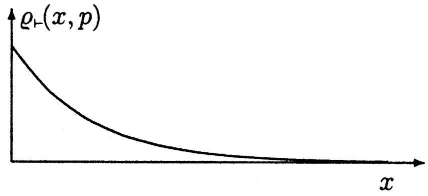


Fig. 2. Typical plot of dislocation density $\varrho_{\vdash}(x,p)$ as a function of $x$ for $p > p_1$.

(Fig. 2). Hence, GNDs accumulate in a boundary layer with characteristic length $L$ at $x = 0$. Further, in this initial stage of plastic deformation the dislocation density at the grain boundary increases linearly with the loading.

(iii) For $p_2 \leqslant p < p_3$,

$$\gamma(x,p) = -r(p) + s(p)e^{-x/L}, \tag{11.15}$$

so that, since $\gamma(0,p) \neq 0$, grain boundary slip is activated. Moreover,

$$\rho_{\vdash}(x,p) = \frac{s(p)\sin\theta}{L}e^{-x/L}, \tag{11.16}$$

and, as in (ii), GNDs accumulate in a boundary layer with characteristic length $L$, but now, as a consequence of softening at the grain boundary, the GND density at $x = 0$ decreases as the loading increases.

(iv) For $p \geqslant p_3$,

$$\gamma(x,p) = -r(p) + s(p_3)e^{-x/L}, \tag{11.17}$$

with $s(p_3) = 2L\bar{\zeta}_0/c\sin^2\theta$, and hence

$$\rho_{\vdash}(x,p) = \frac{s(p_3)\sin\theta}{L}e^{-x/L}. \tag{11.18}$$

In this stage the grain boundary cannot soften further, and the GND density remains constant at the boundary as the loading increases (Fig. 3).

Note that, defining the *average accumulated slip in bulk* as

$$\gamma_{\text{bulk}}(p) = \lim_{R\to\infty}\frac{1}{R}\int_0^R \gamma(x,p)\,dx,$$

the identity

$$r(p) = -\gamma_{\text{bulk}}(p),$$

which follows from (11.13), (11.15) and (11.17), shows that the bulk forcing function measures the accumulated slip in bulk. Analogously, the difference between the grain boundary and bulk forcing functions,

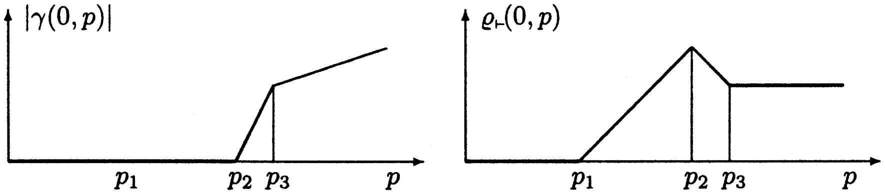


Fig. 3. Variation of accumulated slip $|\gamma(0,p)|$ and dislocation density $\varrho_{\vdash}(0,p)$ at the grain boundary as a function of the loading $p$.

$$s(p) - r(p) = \gamma(0, p), \quad p > p_2,$$

measures the slip accumulated at the interface.

To prove (i), (ii) and (iii), note first that, by (11.4), the displacement gradient and plastic strain tensor have the form

$$\nabla \mathbf{u} = \begin{pmatrix} u_x & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathbf{H}^p = \begin{pmatrix} \gamma \sin\theta & 0 \\ 0 & -\gamma \sin\theta \end{pmatrix}, \tag{11.19}$$

so that, if the elasticity tensor is isotropic, the stress tensor $\mathbf{T} = \lambda\,\mathrm{tr}(\mathbf{E}^e)\mathbf{I} + 2\mu\mathbf{E}^e$ is is given by

$$\mathbf{T} = \begin{pmatrix} (\lambda + 2\mu)u_x - 2\mu\gamma\sin\theta & 0 \\ 0 & \lambda u_x + 2\mu\gamma\sin\theta \end{pmatrix}, \tag{11.20}$$

with $\lambda$ and $\mu$ the Lamé moduli. Inserting this expression into the force balance $\mathrm{div}\,\mathbf{T} = \mathbf{0}$, we obtain the differential equation

$$(\lambda + 2\mu)u_{xx} - 2\mu\gamma_x \sin\theta = 0, \tag{11.21}$$

with the boundary conditions (cf. (11.7))

$$\begin{cases} u = 0 & \text{at } x = 0, \\ (\lambda + 2\mu)u_x - 2\mu\gamma\sin\theta \to -p & \text{as } x \to \infty. \end{cases} \tag{11.22}$$

By (11.21) and $(11.22)_2$,

$$u_x = \frac{1}{\lambda + 2\mu}(2\mu\gamma\sin\theta - p), \tag{11.23}$$

a relation that with $(11.22)_1$ allows us to determine the displacement as a function of the slip $\gamma$.

Consider now the generalized yield conditions (6.2) and (6.3). With the quadratic defect energy (9.9) we have, by (9.6),

$$\boldsymbol{\xi}^\alpha = c(\mathbf{g} \cdot \mathbf{s}^\alpha)\mathbf{s}^\alpha, \quad \mathbf{g} = -\gamma_x \sin\theta \mathbf{e}_2, \tag{11.24}$$

and hence

$$\mathrm{div}\,\boldsymbol{\xi}^1 = -\mathrm{div}\,\boldsymbol{\xi}^2 = \frac{c}{2}\gamma_{xx}\sin^2\theta.$$

From (3.6), (11.3) and (11.21), $\tau^1 = -\tau^2 = \mu\sin\theta(u_x - 2\gamma\sin\theta)$, or equivalently, using (11.23),

$$\tau^1 = -\tau^2 = -\frac{\mu\sin\theta}{\lambda + 2\mu}(2(\lambda + \mu)\gamma\sin\theta + p).$$

Inserting these expressions into (6.2) and (6.3), we obtain the yield conditions

$$-\sigma < \frac{c}{2}\gamma_{xx}\sin^2\theta - \frac{E\sin^2\theta}{2(1 - v^2)}\gamma - \frac{(1 - 2v)\sin\theta}{2(1 - v)}p < \sigma, \quad \dot{\gamma} = 0, \tag{11.25}$$

and

$$\left.\begin{aligned} &\frac{c}{2}\gamma_{xx}\sin^2\theta - \frac{E\sin^2\theta}{2(1 - v^2)}\gamma - \frac{(1 - 2v)\sin\theta}{2(1 - v)}p = +\sigma, \quad \dot{\gamma} \geqslant 0, \\ &\frac{c}{2}\gamma_{xx}\sin^2\theta - \frac{E\sin^2\theta}{2(1 - v^2)}\gamma - \frac{(1 - 2v)\sin\theta}{2(1 - v)}p = -\sigma, \quad \dot{\gamma} \leqslant 0, \end{aligned}\right\} \tag{11.26}$$

with $E$ is Young's modulus and $v$ is Poisson's ratio.

Consider now a monotone increasing loading program $p = p(t) > 0$, with $p(0) = 0$ and $\gamma(x, 0) \equiv 0$. Then for some initial interval of time the elastic-range inequality (11.25) has the form

$$-\sigma_0 < -\frac{(1-2\nu)\sin\theta}{2(1-\nu)}p < \sigma_0, \quad \dot{\gamma} = 0;$$

the solution therefore remains elastic until $p = p_1$, which establishes (i).

When $p = p_1$ the lower yield condition in (11.25) is attained; thus for $p > p_1$ the crystal will flow with $\dot{\gamma} \leqslant 0$, so that

$$\gamma \leqslant 0. \tag{11.27}$$

Thus the grain-boundary relations (10.20) and (10.21), for $i = 2$, take the form

$$\frac{c}{2}\gamma_x(0,p)\sin^2\theta > -\zeta, \quad \dot{\gamma}(0,p) = 0 \tag{11.28}$$

and

$$\frac{c}{2}\gamma_x(0,p)\sin^2\theta = -\zeta, \quad \dot{\gamma}(0,p) \leqslant 0, \tag{11.29}$$

where $\zeta$ evolves according to the softening equation (11.6).

Next, integrating the hardening equation (11.5) we obtain

$$\sigma = -k\gamma + \sigma_0, \tag{11.30}$$

which, when inserted into (11.26), yields the ordinary differential equation

$$\gamma_{xx} - \frac{1}{L^2}(\gamma + r(p)) = 0. \tag{11.31}$$

The associated boundary condition at infinity follows from (11.8) and (11.24):

$$\gamma_x \to 0 \quad \text{as } x \to \infty. \tag{11.32}$$

Since $\gamma(0,p) = 0$ for $p = p_1$, we may conclude from (11.28) that $\gamma(0,p) = 0$ for $p > p_1$ as long as the inequality in (11.28) is satisfied. The solution of (11.31) subject to (11.32) and

$$\gamma(0,p) = 0 \tag{11.33}$$

is (11.13). By (11.28), the solution (11.13) will hold as long as

$$-\frac{cr(p)\sin^2\theta}{2L} > -\zeta_0, \tag{11.34}$$

or equivalently, by $(11.12)_1$, as long as $p < p_2$ with $p_2$ given by $(11.11)_2$. To obtain (11.14), it is sufficient to note that, by (2.4), the GND edge densities of the two slip systems coincide and are proportional to the slip gradient:

$$\rho^1_\vdash = \rho^2_\vdash = -\gamma_x \sin\theta. \tag{11.35}$$

When $p > p_2$, slip is activated at the grain boundary, and $\dot{\gamma}(0,p)$ is no longer required to vanish. The basic equation (11.31) for slip in bulk remains unchanged, as well as the boundary conditions (11.32), but (11.33) is now replaced by the grain boundary condition (11.29):

$$\frac{c}{2}\gamma_x(0,p)\sin^2\theta = -\zeta. \tag{11.36}$$

Integrating the softening equation (11.6) we obtain

$$\zeta = h\gamma + \zeta_0, \tag{11.37}$$

which, when inserted into (11.36), yields

$$\frac{c}{2}\gamma_x(0,p)\sin^2\theta + h\gamma(0,p) + \zeta_0 = 0. \tag{11.38}$$

The solution of (11.31) subject to the boundary conditions (11.38) and (11.32) yields (11.15). Finally, (11.16) follows from (11.35).

The boundary condition (11.38) holds as long as $h\gamma(0,p) + \zeta_0 > \bar{\zeta}_0$. A straightforward computation shows that $\bar{\zeta}_0$ is reached at $p = p_3$, so that, for $p > p_3$, the grain boundary condition (11.36) becomes

$$\frac{c}{2}\gamma_x(0,p)\sin^2\theta = -\bar{\zeta}_0, \tag{11.39}$$

which yields (11.17).

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