On the characterization of geometrically necessary dislocations in finite plasticity

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Abstract

We develop a general theory of geometrically necessary dislocations based on the decomposition $\boldsymbol{F} = \boldsymbol{F}^e\boldsymbol{F}^p$. The incompatibility of $\boldsymbol{F}^e$ and that of $\boldsymbol{F}^p$ are characterized by a single tensor $\boldsymbol{G}$ giving the Burgers vector, measured and reckoned per unit area in the microstructural (intermediate) configuration. We show that G may be expressed in terms of $\boldsymbol{F}^p$ and the referential curl of $\boldsymbol{F}^p$, or *equivalently* in terms of $\boldsymbol{F}^{e-1}$ and the spatial curl of $\boldsymbol{F}^{e-1}$. We derive explicit relations for $\boldsymbol{G}$ in terms of Euler angles for a rigid-plastic material and — without neglecting elastic strains — for strict plane strain and strict anti-plane shear. We discuss the relationship between $\boldsymbol{G}$ and the distortion of microstructural planes. We show that kinematics alone yields a balance law for the transport of geometrically necessary dislocations.

Keywords: A. dislocations, B. crystal plasticity, B. Finite strain.

1 Introduction

Modern treatments of finite plasticity are based on the Kröner-Lee decomposition[1]

$$\boldsymbol{F} = \boldsymbol{F}^e\boldsymbol{F}^p \tag{1.1}$$

of the deformation gradient $\boldsymbol{F} = \nabla\boldsymbol{y}$ into structural (elastic) and plastic components, where $\boldsymbol{x} = \boldsymbol{y}(\boldsymbol{X}, t)$ represents the deformation that carries material points $\boldsymbol{X}$ in the reference configuration into their positions $\boldsymbol{x}$ at time t in the deformed configuration. For a single crystal, $\boldsymbol{F}^p(\boldsymbol{X})$ represents the "local deformation" of *referential* line segments to line segments $d\boldsymbol{l} = \boldsymbol{F}^p(\boldsymbol{X})d\boldsymbol{X}$ in the *microstructural configuration*,[2] a deformation resulting solely from the formation of defects such as dislocations; $\boldsymbol{F}^e(\boldsymbol{X})$ represents the "local deformation" of the segments $d\boldsymbol{l}$ into segments $d\boldsymbol{x} = \boldsymbol{F}^e(\boldsymbol{X})d\boldsymbol{l}$ due to stretching and rotation of the *lattice*.

An important feature of the Kröner-Lee decomposition is that, while $\boldsymbol{F}$ is *compatible* (the gradient of a vector field), $\boldsymbol{F}^e$ and $\boldsymbol{F}^p$ are generally *incompatible*, a property related to the formation of dislocations. Such dislocations are termed *geometrically necessary*, as they arise solely from the underlying kinematics, and their intrinsic characterization is basic to general theories of plasticity.

In crystal physics dislocations may be quantified by the Burgers vector, which represents the closure-deficit of circuits deformed from a perfect lattice, and one may ask whether in a continuum theory it is

[1] Kröner (1960), Lee (1969).
[2] We also use the term lattice configuration when discussing single crystals.

possible to characterize such dislocations through a tensor field $\boldsymbol{G}$ that measures the local Burgers vector per unit area. In fact, the problem is not the absence of such a field, but rather the plethora of fields that have appeared in the literature. Here our central task is to show that there is but a single measure of geometrically necessary dislocations consistent with physically motivated requirements. To place our ideas in context we begin, after fixing notation, with a brief historical discussion of this question.

1.1 Notation for differential operators

Throughout,

$$\nabla, \quad \mathrm{Div}, \quad \text{and} \quad \mathrm{Curl}$$

denote the gradient, divergence, and curl with respect to the material point $\boldsymbol{X}$ in the *reference configuration*;

$$\mathrm{grad}, \quad \mathrm{div}, \quad \text{and} \quad \mathrm{curl}$$

denote the divergence, gradient, and curl with respect to the point $\boldsymbol{x}=\boldsymbol{y}(\boldsymbol{X},t)$ in the *deformed configuration*; given any field φ,

$$\dot{\varphi} \quad \text{and} \quad \frac{\partial\varphi}{\partial t}$$

denote its *material time-derivative* (holding $\boldsymbol{X}$ fixed) and its *spatial time-derivative* (holding $\boldsymbol{x}$ fixed).

1.2 Historical perspective. Critical comments

The early treatments of geometrically necessary dislocations, generally referred to as GNDs, are based on a representation of the crystalline structure by three independent director-fields $\boldsymbol{e}_k(\boldsymbol{x})$. These fields are viewed as the generators, on a microscopic scale, of a Bravais lattice deformed via a tensor field $\boldsymbol{A}(\boldsymbol{x})$ through a transformation $\boldsymbol{e}_k(\boldsymbol{x})=\boldsymbol{A}(\boldsymbol{x})\boldsymbol{c}_k$ of a basis $\boldsymbol{c}_k$ of a fixed reference lattice $\mathcal{L}$. Defectiveness is then measured, in the spirit of Burgers, by quantifying the closure failure of infinitesimal circuits in this microscopic lattice. This point of view is easily reconcilied with the formulation in terms of (1.1) upon identifying the elastic deformation tensor $\boldsymbol{F}^e$ with $\boldsymbol{A}$. This approach to defectiveness is apparently due to Kondo (1952, 1955), who framed his treatment within a differential-geometric framework using the theory of connections with defectiveness characterized by the non-holonomicity of the director fields. His measure of GNDs — the torsion of the connection generated by the director fields — results in a third-order tensor-field that equivalently may be expressed as the second-order tensor-field

$$\boldsymbol{G}^e_{\mathrm{Ko}} = J^e\boldsymbol{F}^{e-1}\mathrm{curl}\,\boldsymbol{F}^{e-1}, \tag{1.2}$$

with $J^e = \det\boldsymbol{F}^e$.[3] At about the same time, and independently, Nye (1953) used physical arguments to justify a formula relating the local Burgers vector to the local rotation of the directors; tacit in Nye's work is the neglect of elastic strains and the assumption of infinitesimal rotations, and his resulting defect measure is

$$\mathrm{curl}\,\boldsymbol{W}^e,$$

with $\boldsymbol{W}^e$ the skew tensor that represents infinitesimal rotations of the lattice. Based on Nye's ideas, Bilby, Bullough, and Smith (1955), Eshelby (1956), Fox (1966), and Acharya and Bassani (2000), respectively, proposed tensor fields essentially equivalent to

$$\mathrm{curl}\,\boldsymbol{F}^e\boldsymbol{F}^{e-\top}, \quad \mathrm{curl}\,\boldsymbol{F}^e, \quad \boldsymbol{F}^{e-1}\mathrm{curl}\,\boldsymbol{F}^{e-1}, \quad \text{and} \quad \boldsymbol{R}^{e\top}\mathrm{curl}\,\boldsymbol{F}^{e-1} \tag{1.3}$$

as measures of GNDs in finite deformations.

An approach essentially different from those described above is that of Kröner (1960), who, based on the decomposition (1.1), introduces the defect measures[4]

$$\boldsymbol{G}^e_{\mathrm{Kr}} = \mathrm{curl}\,\boldsymbol{F}^{e-1}\boldsymbol{F}^{e\top} \qquad \text{and} \qquad \boldsymbol{G}^p_{\mathrm{Kr}} = \mathrm{Curl}\,\boldsymbol{F}^p. \tag{1.4}$$

[3] Teodosiu (1970, 1982) noted that $\boldsymbol{G}^{e\top}_{\mathrm{Ko}}\boldsymbol{n}$ represents the Burgers vector — measured in the reference lattice — for an infinitesimal circuit in $\mathcal{L}$ enclosing a surface element with unit normal $\boldsymbol{n}$. Davini (1986) showed that $\boldsymbol{G}^e_{\mathrm{Ko}}$ is invariant under superposed compatible elastic deformations (cf. Davini and Parry (1989) and Cermelli and Sellers (2000)). Cf. also Noll (1967), who is led to $\boldsymbol{G}^e_{\mathrm{Ko}}$ in his theory of materially uniform simple bodies with inhomogenieties.

[4] $\boldsymbol{G}^p_{\mathrm{Kr}}$ was used by Naghdi & Srinivasa (1993), $\boldsymbol{G}^e_{\mathrm{Kr}}$ by Dłużewski (1996).

Kröner then goes on to develop a complete theory in the context of infinitesimal displacements, where $\boldsymbol{G}^e_{\rm Kr} = \boldsymbol{G}^p_{\rm Kr}$. This is apparently the first instance in which the problem of the equivalence of elastic and plastic defect measures is addressed.

The variety of measures described above — each proposed as a representation of GNDs — begs the question as to which measure(s), if any, have an intrinsic physical meaning. Requirements, not mutually independent, that one might consider as reasonable characterizations of such a measure are that:[5]

(*i*) $\boldsymbol{G}$ should measure the local Burgers vector in the microstructural configuration, per unit area in that configuration;

(*ii*) $\boldsymbol{G}$ should, at any point, be expressible in terms of the *field* $\boldsymbol{F}^p$ *in a neighborhood of the point*, since, by fiat, $\boldsymbol{F}^p$ characterizes the defect structure near the point in question;

(*iii*) $\boldsymbol{G}$ should be invariant under superposed compatible elastic deformations and also under compatible local changes in reference configuration, since these — being compatible — should not result in an *intrinsic* change in the distribution of GNDs near any point.

It is clear from the work of Teodosiu (1970, 1982) and Davini (1986) that the measure $\boldsymbol{G}^e_{\rm Ko}$ satisfies (*i*) and (*iii*), but (*ii*) would seem problematic. On the other hand, $\boldsymbol{G}^p_{\rm Kr}$ trivially satisfies (*ii*), but violates (*i*). The remaining measures listed in (1.3) violate (*i*) and (*iii*).

1.3 The geometric dislocation tensor $\boldsymbol{G}$

Our main result is the existence of a tensorial measure of GNDs, *geometric dislocation tensor* $\boldsymbol{G}$; specifically,

> $\boldsymbol{G}^\top\boldsymbol{n}$ *gives the local Burgers vector in the microstructural configuration — per unit area in that configuration — for those dislocation lines piercing the plane* Π *with unit normal* $\boldsymbol{n}$.

More simply, we refer to $\boldsymbol{G}^\top\boldsymbol{n}$ as *the Burgers vector for* Π. What is most important, $\boldsymbol{G}$ may be expressed in a form[6]

$$\boldsymbol{G} = \frac{1}{J^p}\boldsymbol{F}^p\,\mathrm{Curl}\,\boldsymbol{F}^p \tag{1.5}$$

that depends only on the plastic part $\boldsymbol{F}^p$ of the deformation gradient and *equivalently* in Kondo's form

$$\boldsymbol{G} = J^e\boldsymbol{F}^{e-1}\mathrm{curl}\,\boldsymbol{F}^{e-1}, \tag{1.6}$$

which depends only on the field $\boldsymbol{F}^e$.

The importance of the alternative plastic and elastic representations of $\boldsymbol{G}$ is that:

(*i*) For situations in which lattice strains are small, GNDs would seem amenable to experimental study through measurement of lattice rotations;[7] the relation for $\boldsymbol{G}$ in terms of $\boldsymbol{F}^e$ (in this case a rotation) allows for its experimental study.

(*ii*) In developing a constitutive theory that allows for GNDs, it would seem advantageous to use the representation for $\boldsymbol{G}$ in terms of $\boldsymbol{F}^p$, which characterizes defects, leaving $\boldsymbol{F}^e$ to describe the stretching and rotation of the lattice. The importance of the relation for $\boldsymbol{G}$ in terms of $\boldsymbol{F}^p$ is underlined by a relation we derive giving $\dot{\boldsymbol{G}}$ for a single crystal as a function of $\boldsymbol{F}^p$, $\mathrm{Curl}\,\boldsymbol{F}^p$, the slips, and the slip gradients.

Given a fixed unit vector $\boldsymbol{n}$, consider the microstructural plane Π normal to $\boldsymbol{n}$. We show that $\boldsymbol{n}\cdot\boldsymbol{G}(\boldsymbol{x})\boldsymbol{n}$ — the normal component of the Burgers vector for Π — is related to the *distortion* of Π. Precisely, we show that, $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = 0$ everywhere if and only if Π is *undistorted*; that is, if and only if Π convects to a family of

[5] Note that the conditions (ii) and (iii) trivially render $\boldsymbol{G}$ frame-indifferent; of (1.3), only $(1.3)_{3,4}$ are frame-indifferent.

[6] Because we do *not* require that $\det \boldsymbol{F}^p = 1$, our discussion allows for the formation of voids and the interaction of voids with other defects.

[7] Cf. Sun et. al. (1998, 2000).

smooth surfaces in the deformed configuration. Our proof of this result is based on a classical theorem of Frobenius in conjunction with the equivalence

$$\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = 0 \quad \Leftrightarrow \quad \bar{\boldsymbol{n}}\cdot\mathrm{curl}\,\bar{\boldsymbol{n}} = 0 \tag{1.7}$$

in which $\bar{\boldsymbol{n}}(\boldsymbol{x})$ represents that unit normal field in the deformed configuration to which $\boldsymbol{n}$ convects. We use (1.7) to show that Π is locally undistorted at a given point if and only if $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ vanishes at that point. These results would seem to indicate that the field $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ might be useful as a constitutive quantity related to hardening due to the formation of GNDs.[8]

When elastic strains are negligible, so that $\boldsymbol{F}^e$ is a rotation $\boldsymbol{R}^e$, GNDs are amenable to experimental study through the measurement of lattice rotations as described by $\boldsymbol{R}^e$. Materials scientists typically describe rotations by means of Euler angles via a decomposition of the form

$$\boldsymbol{R}^e = \boldsymbol{Q}_3\boldsymbol{Q}_2\boldsymbol{Q}_1, \qquad \boldsymbol{Q}_i(\boldsymbol{x}) = \boldsymbol{Q}(\vartheta_i(\boldsymbol{x}), \boldsymbol{c}_i)$$

in which the $\boldsymbol{c}_i$ are constant unit vectors and $\boldsymbol{Q}(\vartheta_i(\boldsymbol{x}), \boldsymbol{c}_i)$ represents a counterclockwise rotation about $\boldsymbol{c}_1$ through an angle $\vartheta_i(\boldsymbol{x})$.[9] As one of our main results we show that the geometric dislocation tensor

$$\bar{\boldsymbol{G}} = \boldsymbol{R}^e\boldsymbol{G}\boldsymbol{R}^{e\top}$$

referred to the deformed configuration has the simple form

$$\bar{\boldsymbol{G}} = \sum_{i=1}^{3}\{\bar{\boldsymbol{c}}_i \otimes \mathrm{grad}\,\vartheta_i - (\bar{\boldsymbol{c}}_i\cdot\mathrm{grad}\,\vartheta_i)\mathbf{1}\},$$

with $\bar{\boldsymbol{c}}_i$ the vectors $\boldsymbol{c}_i$ convected to the deformed configuration.

1.4 Strict plane strain and strict anti-plane shear

Two important classes of deformations are plane strain and anti-plane shear in which the matrices of the deformation gradient $\boldsymbol{F}$, in components with respect to an orthonormal basis $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ with $\boldsymbol{e}_3$ the out-of-plane normal, have the respective forms

$$\begin{bmatrix} \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \cdot & \cdot & 1 \end{bmatrix}$$

with entries independent of X_3. We consider generalizations of plane strain and anti-plane shear defined by the requirement that in each case the tensor fields $\boldsymbol{F}^p$ and $\boldsymbol{F}^e$ have a form identical to that of $\boldsymbol{F}$; we use the adjective *strict* to denote these generalizations.

For strict plane strain with $\boldsymbol{e} = \boldsymbol{e}_3$, $\boldsymbol{G}$ is a "pure edge tensor"

$$\boldsymbol{G} = \boldsymbol{e}\otimes\boldsymbol{g}, \qquad \boldsymbol{e}\cdot\boldsymbol{g} = 0,$$

with $\boldsymbol{e}$ the out-of-plane normal and $\boldsymbol{g}$ the principal Burgers vector. A consequence of this relation is that microstructural planes parallel to $\boldsymbol{e}$ are undistorted. Moreover, if the material is rigid-plastic, then, for ϑ^e the rotation angle corresponding to $\boldsymbol{R}^e$, $\boldsymbol{g}$ may be expressed in the simple form

$$\boldsymbol{g} = -\boldsymbol{R}^{e\top}\mathrm{grad}\,\vartheta^e.$$

Thus $\boldsymbol{g}$ rotated to the deformed configuration is normal to surfaces $\vartheta^e = constant$.

For strict anti-plane shear,

$$\boldsymbol{F}^p = \mathbf{1} + \boldsymbol{e}\otimes\boldsymbol{\gamma}^p,$$

[8]This field, which we term the "distortion modulus", accounts for the normal component of the Burgers vector of those dislocations impinging transversally Π. When Π is a slip plane, these are traditionally termed "forest dislocations" and are thought to be responsible for stage II hardening (Kuhlmann-Wilsdorf 1989).

[9]The standard Euler-angle representation is obtained by choosing $\boldsymbol{c}_1 = \boldsymbol{c}_3 = \boldsymbol{k}$ and $\boldsymbol{c}_2 = \boldsymbol{i}$, with $(\boldsymbol{i}, \boldsymbol{j}, \boldsymbol{k})$ an orthogonal basis; in this case the angles are generally denoted by $\vartheta_3 = \varphi_1$, $\vartheta_2 = \psi$, $\vartheta_1 = \varphi_2$,

with γ^p orthogonal to e, and the geometric dislocation tensor is a "pure screw-tensor"

$$G = e \otimes h$$

with principal Burgers vector

$$h = \operatorname{curl} \gamma^p$$

parallel to e. Microstructural planes perpendicular to e are therefore distorted at any point at which $\operatorname{curl} \gamma^p \neq 0$.

1.5 Dynamics

Kinematics alone yields a balance law for the transport of GNDs. Consider a prescribed microstructural plane Π with unit normal ℓ and a prescribed unit vector b, which need bear no relation to ℓ. We consider $\rho(\ell, b) = \ell \cdot Gb$ — which is the component in the direction b of the Burgers vector, per unit area, on Π — as a "signed density".[10] We show that $\rho = \rho(\ell, b)$ evolves in accord with the *balance law*

$$\dot{\rho} = -\operatorname{Div} q_{\mathrm{R}} + \sigma_{\mathrm{R}},$$

with dislocation flux q_{R} and dislocation supply σ_{R} defined by

$$q_{\mathrm{R}} = F^{p-1}(\ell \times) L^{p\top} b, \qquad \sigma_{\mathrm{R}} = \ell \cdot L^p G b + b \cdot L^p G \ell.$$

This balance is one of our main results; one of its more interesting consequences is that plastic flow, as characterized by nonvanishing values of L^p, is always associated with a flux of dislocations, whether or not G vanishes.[11]

Finally, we derive expressions for single crystals showing the explicit relationship of $\dot{G}$ to the slips (microshear rates) and their gradients.

1.6 The invariant nature of G as a descriptor of GNDs

To underline the intrinsic nature of G as an intrinsic measure of GNDs, we consider functions of the form

$$\Phi = \Phi(F^p, \nabla F^p).$$

If Φ — with values associated solely with the lattice configuration — is to provide an intrinsic characterization of GNDs, then Φ should be invariant under arbitrary *compatible* changes in reference configuration, since such changes should not induce additional GNDs. A central result of ours is that, for Φ to display this invariance, it is both necessary and sufficient that Φ reduce to a function of the form[12]

$$\Phi = \Phi(G).$$

Thus — in contrast to the standard prejudice that constitutive dependences on F^p are unsound — gradient theories meant to characterize GNDs should allow for a dependence on F^p through its presence in the geometric dislocation tensor G.

[10] An alternative approach to the modeling of dislocations has been suggested by Nye (1953). Noting that the Burgers vectors of a single dislocation in a crystal must belong to a well-defined crystallographically determined set, dislocations are accounted for by assigning independent densities of screw and edge type, each corresponding to dislocations with a given Burgers vector in this set. These elementary dislocations may be combined to form the tensor G, but G does not uniquely characterize the elementary densities. For instance, in the "fcc-deconstruction" (Sun et al. 1998, 2000) there are 36 elementary densities, but only 9 independent components of G, a difficulty overcome by a minimization technique that furnishes a lower bound for the total density.

[11] G accounts only only for GNDs, as it measures the *net* dislocation density associated with macroscopic incompatibility.

[12] This theorem was in some ways motivated by a result of Davini (1986), who showed that a function $\Phi(F^{e-1}, \operatorname{curl} F^{e-1})$ is invariant under superposed elastic deformations if and only if Φ reduces to a function of $(\det F^e) F^{e-1} \operatorname{curl} F^{e-1}$.

2 Preliminaries

2.1 Mappings of surfaces

Let $\boldsymbol{h}$ be a smooth one-to-one mapping of a region D_1 of $\mathbb{R}^3$ onto another such region D_2, with

$$\boldsymbol{H} = \nabla \boldsymbol{h}, \qquad \det \boldsymbol{H} > 0. \tag{2.1}$$

Further, let $S_i \subset D_i$ $(i = 1, 2)$ be smooth surfaces with

$$S_2 = \boldsymbol{h}(S_1),$$

and with S_i oriented by a smooth unit-normal field $\boldsymbol{n}_i$. Then, modulo a change in the sign of $\boldsymbol{n}_2$,

$$\boldsymbol{n}_2 = \frac{\boldsymbol{H}^{-\top}\boldsymbol{n}_1}{|\boldsymbol{H}^{-\top}\boldsymbol{n}_1|}, \tag{2.2}$$

where $\boldsymbol{H}^{-\top} = (\boldsymbol{H}^{\top})^{-1}$. The **surface jacobian** of $\boldsymbol{h}$ as a mapping of S_1 onto S_2 is given by

$$\jmath = (\det \boldsymbol{H})|\boldsymbol{H}^{-\top}\boldsymbol{n}_1|, \tag{2.3}$$

so that, for f a scalar field and $\boldsymbol{T}$ a tensor field,[13]

$$\int_{S_2} f\, dA_2 = \int_{S_1} f \jmath\, dA_1, \qquad \int_{S_2} \boldsymbol{T}\boldsymbol{n}_2\, dA_2 = \int_{S_1} (\det \boldsymbol{H})\boldsymbol{T}\boldsymbol{H}^{-\top}\boldsymbol{n}_1\, dA_1, \tag{2.4}$$

with dA_i the area measure on S_i. (The identity $(2.4)_2$ follows from (2.2), (2.3), and $(2.4)_1$.) We refer to the vector measures $\boldsymbol{n}_i\, dA_i$ $(i = 1, 2)$ as **surface elements** with unit normal $\boldsymbol{n}_i$ and area dA_i.

REMARK. We view (2.4), formally, as asserting that the surface element $\boldsymbol{n}_1\, dA_1$ on S_1 is mapped by $\boldsymbol{h}$ into the surface element

$$\boldsymbol{n}_2\, dA_2 = (\det \boldsymbol{H})\boldsymbol{H}^{-\top}\boldsymbol{n}_1\, dA_1 \tag{2.5}$$

on S_2 (with area element dA_1 mapped into $dA_2 = \jmath\, dA_1$ and $\boldsymbol{n}_1$ mapped into $\boldsymbol{n}_2$ via (2.2)).

2.2 The curl operator. Stokes theorem

2.2.1 Definitions. Basic results

The **curl** of a tensor field $\boldsymbol{T}$ is the *tensor* field defined by

$$(\mathrm{curl}\, \boldsymbol{T})\mathbf{c} = \mathrm{curl}\, (\boldsymbol{T}^{\top}\mathbf{c}) \quad \text{for all constant vectors } \mathbf{c}.$$

Let Γ be the boundary curve of a smooth surface S oriented by a continuous unit normal field $\boldsymbol{n}$, with the boundary curve Γ oriented in a manner consistent with Stokes' theorem for smooth vector fields $\boldsymbol{f}$:

$$\int_{\Gamma} \boldsymbol{f} \cdot d\boldsymbol{x} = \int_S (\mathrm{curl}\, \boldsymbol{f}) \cdot \boldsymbol{n}\, dA. \tag{2.6}$$

We then have **Stokes' theorem for a tensor field** $\boldsymbol{T}$:

$$\int_{\Gamma} \boldsymbol{T} d\boldsymbol{x} = \int_S (\mathrm{curl}\, \boldsymbol{T})^{\top}\boldsymbol{n}\, dA. \tag{2.7}$$

The verification of (2.7) is immediate: simply apply (2.6) with $\boldsymbol{f} = \boldsymbol{T}^{\top}\mathbf{c}$ and $\mathbf{c}$ constant.

When convenient we use the standard notation of cartesian tensor analysis — including summation convention — with respect to the basis $\boldsymbol{e}_1 = (1, 0, 0)$, $\boldsymbol{e}_2 = (0, 1, 0)$, $\boldsymbol{e}_3 = (0, 0, 1)$. In particular, the component form of $\mathrm{curl}\, \boldsymbol{T}$ is given by

$$(\mathrm{curl}\, \boldsymbol{T})_{ij} = \epsilon_{irs}\frac{\partial T_{js}}{\partial x_r},$$

with ϵ_{irs} the alternating symbol.[14]

[13] More precisely, if the domain of $\boldsymbol{T}$ is D_1, then the integral over D_2 should involve the composition $\boldsymbol{T} \circ \boldsymbol{h}$; similarly for f.
[14] A cautonary note: for some authors the curl of $\boldsymbol{T}$ is the transpose of our curl$\boldsymbol{T}$.

2.2.2 Transformation law for curl

In terms of the notation introduced in Subsection 2.1, let curl_i denote the curl operator with respect to an arbitrary point $\boldsymbol{x}_i$ in D_i $(i = 1,2)$. Let $S_i \subset D_i$ $(i = 1,2)$ be smooth surfaces with $S_2 = \boldsymbol{h}(S_1)$; let S_i be oriented by a smooth unit-normal field $\boldsymbol{n}_i$ with (2.2) tacit; let Γ_i be the boundary curve of S_i with orientation consistent with Stokes' theorem. Then for $\boldsymbol{f}_2$ a smooth vector field on D_2,

$$\int_{\Gamma_2} \boldsymbol{f}_2 \cdot d\boldsymbol{x}_2 = \int_{S_2} (\mathrm{curl}_2 \boldsymbol{f}_2) \cdot \boldsymbol{n}_2 \, dA_2. \tag{2.8}$$

On the other hand, since $d\boldsymbol{x}_2 = \boldsymbol{H} d\boldsymbol{x}_1$, if we define $\boldsymbol{f}_1(\boldsymbol{x}_1) = \boldsymbol{H}(\boldsymbol{x}_1)^{\top} \boldsymbol{f}_2(\boldsymbol{h}(\boldsymbol{x}_1))$, then

$$\begin{aligned}\int_{\Gamma_2} \boldsymbol{f}_2 \cdot d\boldsymbol{x}_2 = \int_{\Gamma_1} \boldsymbol{f}_1 \cdot d\boldsymbol{x}_1 &= \int_{S_1} (\mathrm{curl}_1 \boldsymbol{f}_1) \cdot \boldsymbol{n}_1 \, dA_1 \\ &= \int_{S_2} (\mathrm{curl}_1 \boldsymbol{f}_1) \cdot \frac{1}{\det \boldsymbol{H}} \boldsymbol{H}^{\top} \boldsymbol{n}_2 \, dA_2 = \int_{S_2} \Big(\frac{1}{\det \boldsymbol{H}} \boldsymbol{H} \mathrm{curl}_1 \boldsymbol{f}_1 \Big) \cdot \boldsymbol{n}_2 \, dA_2.\end{aligned}$$

Thus, since S_2 may be arbitrarily chosen, we have the **transformation law**

$$\mathrm{curl}_2 \boldsymbol{f}_2 = \frac{1}{\det \boldsymbol{H}} \boldsymbol{H} \, \mathrm{curl}_1 \boldsymbol{f}_1, \qquad \boldsymbol{f}_2 = \boldsymbol{H}^{-\top} \boldsymbol{f}_1. \tag{2.9}$$

A consequence of (2.9) is that, for $\boldsymbol{T}_2$ a smooth tensor field on D_2,

$$\mathrm{curl}_2 \boldsymbol{T}_2 = \frac{1}{\det \boldsymbol{H}} \boldsymbol{H} \, \mathrm{curl}_1 \boldsymbol{T}_1, \qquad \boldsymbol{T}_2 = \boldsymbol{T}_1 \boldsymbol{H}^{-1}. \tag{2.10}$$

Indeed, for $\boldsymbol{c}$ constant,

$$\{\mathrm{curl}_2 \boldsymbol{T}_2\} \boldsymbol{c} = \mathrm{curl}_2 (\boldsymbol{T}_2^{\top} \boldsymbol{c}) = \frac{1}{\det \boldsymbol{H}} \boldsymbol{H} \, \mathrm{curl}_1 (\boldsymbol{H}^{\top} \boldsymbol{T}_2^{\top} \boldsymbol{c}) = \frac{1}{\det \boldsymbol{H}} \{\boldsymbol{H} \, \mathrm{curl}_1 \boldsymbol{T}_1\} \boldsymbol{c}.$$

2.3 General identities. The skew tensor $\boldsymbol{w}\times$

For $\boldsymbol{e}$ a unit vector, the tensor

$$\mathbb{P}(\boldsymbol{e}) = \mathbf{1} - \boldsymbol{e} \otimes \boldsymbol{e} \tag{2.11}$$

is the **projection** onto the plane perpendicular to $\boldsymbol{e}$, while $\boldsymbol{e}^{\perp}$ denotes the *plane* perpendicular to $\boldsymbol{e}$.

Given any vector $\boldsymbol{w}$, $\boldsymbol{w}\times$ is the *skew tensor* defined by

$$(\boldsymbol{w}\times)\boldsymbol{c} = \boldsymbol{w} \times \boldsymbol{c} \quad \text{for all vectors } \boldsymbol{c};$$

in components $(\boldsymbol{w}\times)_{ij} = \epsilon_{irj} w_r$. Then

$$(\boldsymbol{w}\times)(\boldsymbol{u}\times) = \boldsymbol{u} \otimes \boldsymbol{w} - (\boldsymbol{u} \cdot \boldsymbol{w}) \mathbf{1}, \tag{2.12}$$

so that, for $|\boldsymbol{w}| = 1$, $(\boldsymbol{w}\times)(\boldsymbol{w}\times) = -\mathbb{P}(\boldsymbol{w})$. Given any *skew* tensor $\boldsymbol{W}$, there is a unique vector $\boldsymbol{w}$ such that

$$\boldsymbol{W} = \boldsymbol{w}\times;$$

$\boldsymbol{w}$ is called the **axial vector** of $\boldsymbol{W}$.

IDENTITIES. *Let ν be a scalar field, let $\boldsymbol{f}$ and $\boldsymbol{u}$ be vector fields, let $\boldsymbol{S}$ and $\boldsymbol{T}$ be tensor fields with $\boldsymbol{T}$ constant, and let $\boldsymbol{a}$ be a constant vector. Then*

$$\left.\begin{aligned} \mathrm{curl}\, \nabla \boldsymbol{f} &= \mathbf{0}, \\ \mathrm{curl}\,(\boldsymbol{T}\boldsymbol{S}) &= (\mathrm{curl}\, \boldsymbol{S}) \boldsymbol{T}^{\top}, \\ \mathrm{curl}\,(\nu \boldsymbol{T}) &= (\nabla \nu \times) \boldsymbol{T}^{\top}, \\ \boldsymbol{a} \cdot \mathrm{curl}\, \boldsymbol{f} &= (\boldsymbol{a}\times) \cdot \nabla \boldsymbol{f}, \\ \mathrm{curl}\,(\boldsymbol{u} \otimes \boldsymbol{f}) &= (\mathrm{curl}\, \boldsymbol{f}) \otimes \boldsymbol{u} - (\boldsymbol{f}\times)(\nabla \boldsymbol{u})^{\top}, \\ \mathrm{curl}\,(\boldsymbol{f}\times) &= (\mathrm{div}\, \boldsymbol{f}) \mathbf{1} - \nabla \boldsymbol{f}. \end{aligned}\right\} \tag{2.13}$$

Moreover, if rather than being a constant, $\boldsymbol{T}(\nu)$ is a function of ν, then

$$\operatorname{curl}(\boldsymbol{TS}) = (\operatorname{curl}\boldsymbol{S})\boldsymbol{T}^{\top} + (\nabla\nu\times)(\frac{d\boldsymbol{T}}{d\nu}\boldsymbol{S})^{\top}. \tag{2.14}$$

Proof. For $\boldsymbol{c}$ a constant vector,

$$(\operatorname{curl}\nabla\boldsymbol{f})\boldsymbol{c} = \operatorname{curl}\{(\nabla\boldsymbol{f})^{\top}\boldsymbol{c}\} = \operatorname{curl}\nabla(\boldsymbol{f}\cdot\boldsymbol{c}) = \boldsymbol{0},$$
$$\{\operatorname{curl}(\boldsymbol{TS})\}\boldsymbol{c} = \operatorname{curl}\{\boldsymbol{S}^{\top}(\boldsymbol{T}^{\top})\boldsymbol{c})\} = (\operatorname{curl}\boldsymbol{S})\boldsymbol{T}^{\top}\boldsymbol{c},$$
$$\{\operatorname{curl}(\nu\boldsymbol{T})\}\boldsymbol{c} = \operatorname{curl}(\nu\boldsymbol{T}^{\top}\boldsymbol{c}) = (\nabla\nu\times)\boldsymbol{T}^{\top}\boldsymbol{c},$$

which verifies $(2.13)_{1-3}$. The identity $(2.13)_4$ follows from the definitions of curl and $\boldsymbol{a}\times$. The identity $(2.13)_5$ follows from the computation

$$\{\operatorname{curl}(\boldsymbol{u}\otimes\boldsymbol{f})\}\boldsymbol{c} = \operatorname{curl}\{(\boldsymbol{c}\cdot\boldsymbol{u})\boldsymbol{f}\} = (\boldsymbol{c}\cdot\boldsymbol{u})(\operatorname{curl}\boldsymbol{f}) - \boldsymbol{f}\times\nabla(\boldsymbol{c}\cdot\boldsymbol{u}) = \{(\operatorname{curl}\boldsymbol{f})\otimes\boldsymbol{u} - (\boldsymbol{f}\times)(\nabla\boldsymbol{u})^{\top}\}\boldsymbol{c},$$

while $(2.13)_6$ is a consequence of the relation $\{\operatorname{curl}(\boldsymbol{f}\times)\}\boldsymbol{c}=\operatorname{curl}(\boldsymbol{c}\times\boldsymbol{f})$ and standard vector identities.

Assume next that $\boldsymbol{T} = \boldsymbol{T}(\nu)$. The curl of $\boldsymbol{TS}$ is the curl holding $\boldsymbol{T}$ fixed plus the curl holding $\boldsymbol{S}$ fixed. Denoting the latter by $\operatorname{curl}_{\boldsymbol{T}}$, we may use $(2.13)_2$ to conclude that

$$\operatorname{curl}(\boldsymbol{TS}) = (\operatorname{curl}\boldsymbol{S})\boldsymbol{T}^{\top} + \operatorname{curl}_{\boldsymbol{T}}(\boldsymbol{TS}).$$

Further, for $\boldsymbol{c}$ a constant vector,

$$\{\operatorname{curl}_{\boldsymbol{T}}(\boldsymbol{TS})\}\boldsymbol{c} = \operatorname{curl}_{\boldsymbol{T}}\{(\boldsymbol{TS})^{\top}\boldsymbol{c}\} = (\nabla\nu\times)(\frac{d\boldsymbol{T}}{d\nu}\boldsymbol{S})^{\top}\boldsymbol{c},$$

so that $\operatorname{curl}_{\boldsymbol{T}}(\boldsymbol{TS}) = (\nabla\nu\times)(\frac{d\boldsymbol{T}}{d\nu}\boldsymbol{S})^{\top}$, which yields (2.14). This completes the proof.

A tensor $\boldsymbol{T}$ that satisfies

$$\boldsymbol{Te} = \boldsymbol{0} \qquad \text{and} \qquad \boldsymbol{T}^{\top}\boldsymbol{e} = \boldsymbol{0},$$

so that $\boldsymbol{T} = \mathbb{P}(\boldsymbol{e})\boldsymbol{T}\,\mathbb{P}(\boldsymbol{e})$, is said to be **essentially from $\boldsymbol{e}^{\perp}$ to $\boldsymbol{e}^{\perp}$**. An example of such a tensor is $\boldsymbol{e}\times$, and since $\boldsymbol{e}\times$ is skew and $\mathbb{P}(\boldsymbol{e})$ symmetric, we have the identity

$$(\boldsymbol{e}\times)\cdot\boldsymbol{S} = (\boldsymbol{e}\times)\cdot\{\mathbb{P}(\boldsymbol{e})\boldsymbol{S}\,\mathbb{P}(\boldsymbol{e})\} = (\boldsymbol{e}\times)\cdot\operatorname{skw}\{\mathbb{P}(\boldsymbol{e})\boldsymbol{S}\,\mathbb{P}(\boldsymbol{e})\} \tag{2.15}$$

for any tensor $\boldsymbol{S}$. Here and in what we follows we define the symmetric and skew parts of a tensor $\boldsymbol{A}$ by

$$\operatorname{sym}\boldsymbol{A} = \tfrac{1}{2}(\boldsymbol{A} + \boldsymbol{A}^{\top}), \qquad \operatorname{skw}\boldsymbol{A} = \tfrac{1}{2}(\boldsymbol{A} - \boldsymbol{A}^{\top}).$$

Finally, since

$$(\det\boldsymbol{T})\epsilon_{ijk} = \epsilon_{pqr}T_{ip}T_{jq}T_{kr},$$

it follows that, for $\boldsymbol{T}$ invertible,

$$\boldsymbol{T}(\boldsymbol{b}\times)\boldsymbol{T}^{\top} = (\det\boldsymbol{T})\,(\boldsymbol{T}^{-\top}\boldsymbol{b})\times\ . \tag{2.16}$$

3 Basic kinematics

3.1 Macroscopic kinematics

Consider a body $\mathrm{B_R}$ identified with the open region of space it occupies in a fixed reference configuration, and assume that, in this configuration, $\mathrm{B_R}$ is homogeneous, although possibly defective.

Let $\boldsymbol{X}$ denote an arbitrary material point of $\mathrm{B_R}$. Assume that the body is evolving, but fix the time and suppress it in what follows. A **motion** of $\mathrm{B_R}$ (at that time) is then a smooth one-to-one mapping

$$\boldsymbol{x} = \boldsymbol{y}(\boldsymbol{X})$$

with **deformation gradient**

$$\boldsymbol{F} = \nabla\boldsymbol{y} \tag{3.1}$$

consistent with

$$J = \det\boldsymbol{F} > 0.$$

3.2 Plastic strain. Structural deformation tensor

The *conceptual hypothesis* underlying the theory is that there is a "microscopic structure" — a lattice in the case of a single crystal — with respect to which microscopic kinematical hypotheses can be framed. Specifically, the theory is based on the decomposition

$$\boldsymbol{F} = \boldsymbol{F}^e \boldsymbol{F}^p, \tag{3.2}$$

where $\boldsymbol{F}^p$, the **plastic strain**, represents the evolution of material through this microscopic structure due to the flow of defects, while $\boldsymbol{F}^e$, the **structural deformation tensor**, represents *stretching and rotation* of the microscopic structure. Unlike $\boldsymbol{F}$, the tensors $\boldsymbol{F}^p$ and $\boldsymbol{F}^e$ do not generally correspond to deformations (i.e., are not gradients of vector fields), but because $\boldsymbol{F}^p$ and $\boldsymbol{F}^e$ are invertible, we may view these tensors as deformations of infinitesimal neighborhoods. We use the term **microstructural configuration** — or **lattice configuration** in the case of a single crystal — for the collection of infinitesimal configurations obtained by applying $\boldsymbol{F}^p$ locally to reference increments $d\boldsymbol{X}$ or, equivalently, by applying $\boldsymbol{F}^{e-1}$ locally to increments $d\boldsymbol{x}$. By (3.2),

$$J = J^e J^p, \qquad J^e = \det \boldsymbol{F}^e, \qquad J^p = \det \boldsymbol{F}^p, \tag{3.3}$$

and we assume, without loss in generality, that

$$J^e > 0, \qquad J^p > 0.$$

For specificity, we consider the microstructural fields $\boldsymbol{F}^e$, $\boldsymbol{F}^p$, J^e, and J^p as functions of $\boldsymbol{X}$ on B_R.

The tensor field $\boldsymbol{L}^p$ defined by the relation

$$\dot{\boldsymbol{F}}^p = \boldsymbol{L}^p \boldsymbol{F}^p \tag{3.4}$$

represents the **plastic strain-rate**, measured in the microstructural configuration. A standard identity then yields an analogous relation for J^p:

$$\dot{J}^p = J^p \,\mathrm{tr} \boldsymbol{L}^p. \tag{3.5}$$

Particular microscopic structures are often characterized by restrictions on the form of the tensor $\boldsymbol{L}^p$.

The polar decompositions

$$\left.\begin{aligned} \boldsymbol{F}^p &= \boldsymbol{R}^p \boldsymbol{U}^p = \boldsymbol{V}^p \boldsymbol{R}^p, \\ \boldsymbol{F}^e &= \boldsymbol{R}^e \boldsymbol{U}^e = \boldsymbol{V}^e \boldsymbol{R}^e \end{aligned}\right\} \tag{3.6}$$

define the plastic and elastic rotations $\boldsymbol{R}^p$ and $\boldsymbol{R}^e$, the plastic and elastic right-stretch tensors $\boldsymbol{U}^p$ and $\boldsymbol{U}^e$, and the plastic and elastic left-stretch tensors $\boldsymbol{V}^p$ and $\boldsymbol{V}^e$. A case of special interest corresponds to situations in which the microscopic structure may be treated as rigid, so that the sole source of local deformation is due to the flow of defects. Such materials — referred to as **rigid-plastic** — are defined by the restriction

$$\boldsymbol{U}^e = \boldsymbol{V}^e = \boldsymbol{1}, \qquad (\text{so that } \ \boldsymbol{F}^e = \boldsymbol{R}^e, \ \ J^e = 1). \tag{3.7}$$

3.3 Convection of geometric quantities

We use the term **convect** to indicate the manner in which geometrical objects "deform" during the motion. Thus the **reference body** B_R convects to the **deformed body**

$$\bar{\mathrm{B}} \stackrel{\text{def}}{=} \boldsymbol{y}(\mathrm{B}_\mathrm{R});$$

an oriented surface S_R with unit normal $\boldsymbol{n}_\mathrm{R}$ convects to the oriented surface $\bar{S} = \boldsymbol{y}(S_\mathrm{R})$ with unit normal

$$\bar{\boldsymbol{n}} = \frac{\boldsymbol{F}^{-\top} \boldsymbol{n}_\mathrm{R}}{|\boldsymbol{F}^{-\top} \boldsymbol{n}_\mathrm{R}|} \tag{3.8}$$

(cf.(2.2)); the surface element $\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}}$ on S_{R} convects to the surface element $\bar{\boldsymbol{n}}\,d\bar{A}$ on $\bar{S}$ defined by

$$\bar{\boldsymbol{n}}\,d\bar{A} = J\boldsymbol{F}^{-\top}\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}} \tag{3.9}$$

(cf. the Remark in Subsection 2.1).

Consistent with this, we use the following notation for a *geometrical object* $\{\dots\}$ (such as a unit normal field) that may be described relative to some or all of the underlying configurations:

(a) $\{\dots\}_{\mathrm{R}}$ denotes its representation in the reference configuration;

(b) $\{\dots\}$ (no embellishments) denotes its representation in the microstructural configuration;

(c) $\overline{\{\dots\}}$ denotes its representation in the deformed configuration.

We use this scheme even when the quantity has no representation in the microstructural configuration (e.g., B_{R} is the reference body and $\bar{\mathrm{B}}$ is the deformed body), but in each case the quantities will be consistent with our use of the term "convect" in the sense that $\{\dots\}$ **convects from** $\{\dots\}_{\mathrm{R}}$ and **convects to** $\overline{\{\dots\}}$, and so forth.

The ambient space of the microstructural configuration consists of a collection of copies of $\mathbb{R}^3$, one copy $\mathcal{L}(\boldsymbol{X})$ for each material point $\boldsymbol{X}$. $\mathcal{L}(\boldsymbol{X})$ should be viewed the ambient space into which an infinitesimal neighborhood of $\boldsymbol{X}$ is carried by the linear transformation $\boldsymbol{F}^p(\boldsymbol{X})$ — or from which an infinitesimal neighborhood of $\boldsymbol{x}=\boldsymbol{y}(\boldsymbol{X})$ is carried backwards by $\boldsymbol{F}^{e-1}(\boldsymbol{x})$.[15] The operation of integration is physically meaningless on $\mathcal{L}(\boldsymbol{X})$, as integration is *not local*, but the notion of a surface element $\boldsymbol{n}\,dA$ (with unit normal $\boldsymbol{n}$ and area dA) does have meaning, as $\boldsymbol{n}\,dA$ is *local*. Thus, bearing in mind the Remark in Subsection 2.1, we *formally* stipulate that a unit normal $\boldsymbol{n}_{\mathrm{R}}$ and surface element $\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}}$ at $\boldsymbol{X}$ convect to the unit normal

$$\boldsymbol{n} = \frac{\boldsymbol{F}^{p-\top}\boldsymbol{n}_{\mathrm{R}}}{|\boldsymbol{F}^{p-\top}\boldsymbol{n}_{\mathrm{R}}|} \tag{3.10}$$

and surface element

$$\boldsymbol{n}\,dA = J^p\boldsymbol{F}^{p-\top}\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}} \tag{3.11}$$

in $\mathcal{L}(\boldsymbol{X})$, and that $\boldsymbol{n}$ and $\boldsymbol{n}\,dA$ convect to the unit normal and surface element

$$\bar{\boldsymbol{n}} = \frac{\boldsymbol{F}^{e-\top}\boldsymbol{n}}{|\boldsymbol{F}^{e-\top}\boldsymbol{n}|} \tag{3.12}$$

and

$$\bar{\boldsymbol{n}}\,d\bar{A} = J^e\boldsymbol{F}^{e-\top}\boldsymbol{n}\,dA \tag{3.13}$$

at $\boldsymbol{x}$ in the deformed configuration. Since $\boldsymbol{F}=\boldsymbol{F}^e\boldsymbol{F}^p$, (3.11) and (3.13) are consistent with (3.9).[16]

3.4 Single crystals. Slip

A microscopic structure of particular importance is a single crystal. In this case we restrict attention to plastic flow induced by the motion of dislocations on prescribed slip systems $\alpha=1,2,\dots,A$, with each system α defined by a **slip direction** $\boldsymbol{s}^\alpha$ and a **slip-plane normal** $\boldsymbol{m}^\alpha$, where

$$\boldsymbol{s}^\alpha\cdot\boldsymbol{m}^\alpha = 0, \qquad |\boldsymbol{s}^\alpha|,\,|\boldsymbol{m}^\alpha| = 1, \qquad \boldsymbol{s}^\alpha,\boldsymbol{m}^\alpha = \text{constant}. \tag{3.14}$$

The plane with normal $\boldsymbol{m}^\alpha$ and the line on this plane defined by $\boldsymbol{s}^\alpha$ then represent the **slip plane** and the **slip line** for α, and the tensor

$$\mathbb{S}^\alpha = \boldsymbol{s}^\alpha\otimes\boldsymbol{m}^\alpha \tag{3.15}$$

[15] Throughout, we use abbreviations such as $\boldsymbol{F}^{e-1}=(\boldsymbol{F}^e)^{-1}$ and $\boldsymbol{F}^{p-\top}=(\boldsymbol{F}^p)^{-\top}$.

[16] It suffices to consider the relations (3.11) and (3.13) as formal, as we shall use them only to make meaningful the notion of a tensorial density measured per unit area in the lattice configuration.

is referred to as the **Schmid tensor** for α.

The presumption that flow take place through slip manifests itself in the requirement that the evolution of $\boldsymbol{F}^p$ be governed by **slips** (microshear-rates) ν^α on the individual slip systems via the flow rule

$$\boldsymbol{L}^p = \sum_{\alpha=1}^{A} \nu^\alpha (\boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha) = \sum_{\alpha=1}^{A} \nu^\alpha \mathbb{S}^\alpha. \tag{3.16}$$

By $(3.14)_1$ and (3.16),

$$\mathrm{tr}\boldsymbol{L}^p = 0$$

and a consequence of the differential equation (3.5) is that $J^p = 1$ for all time if $J^p = 1$ initially.

3.5 Isochoric $\boldsymbol{F}^p$. Decomposition for $\boldsymbol{F}^p$ non-isochoric

To characterize internal damage due solely to the formation of voids one might restrict the plastic strain to a **dilatation**:[17]

$$\boldsymbol{F}^p = \lambda^{-1}\mathbf{1}, \qquad J^p = \lambda^{-3}. \tag{3.17}$$

In this case, (3.4) yields the flow rule

$$\boldsymbol{L}^p = \upsilon\mathbf{1}, \qquad \upsilon = -\dot{\overline{\ln\lambda}}. \tag{3.18}$$

An arbitrary plastic strain $\boldsymbol{F}^p$ may be decomposed into the product

$$\boldsymbol{F}^p = \lambda^{-1}\boldsymbol{F}_0^p, \qquad J^p = \lambda^{-3}, \tag{3.19}$$

of a dilatation $\lambda^{-1}\mathbf{1}$ and a plastic strain $\boldsymbol{F}_0^p$ that is **isochoric** in the sense that

$$\det\boldsymbol{F}_0^p = 1. \tag{3.20}$$

Then, by (3.4), the plastic flow, as represented by $\boldsymbol{L}^p$, admits the *additive* decomposition

$$\boldsymbol{L}^p = \upsilon\mathbf{1} + \boldsymbol{L}_0^p,$$

into dilatational and isochoric flows as represented by $\upsilon\mathbf{1}$, $\upsilon = -\dot{\overline{\ln\lambda}}$, and

$$\boldsymbol{L}_0^p = \dot{\boldsymbol{F}}_0^p \boldsymbol{F}_0^{p-1}, \qquad \mathrm{tr}\boldsymbol{L}_0^p = 0.$$

This decomposition with $\boldsymbol{L}_0^p$ in the form (3.16) would represent the *interaction of slip with void-formation in single crystals.*

3.6 Plane strain. Strict plane strain

Under **plane strain** the deformation $\boldsymbol{x} = \boldsymbol{y}(\boldsymbol{X})$ has the component form

$$x_i = y_i(X_1, X_2) \quad (i = 1, 2), \qquad x_3 = X_3.$$

Writing

$$\boldsymbol{e} \equiv \boldsymbol{e}_3,$$

plane strain results in a deformation gradient $\boldsymbol{F}$ and a velocity gradient $\boldsymbol{L}$ that are independent of X_3 and consistent with

$$\left.\begin{aligned} \boldsymbol{F} &= \mathbb{P}(\boldsymbol{e})\boldsymbol{F}\,\mathbb{P}(\boldsymbol{e}) + \boldsymbol{e}\otimes\boldsymbol{e}, \\ \boldsymbol{L} &= \mathbb{P}(\boldsymbol{e})\boldsymbol{L}\,\mathbb{P}(\boldsymbol{e}), \end{aligned}\right\} \tag{3.21}$$

[17]The use of λ^{-1} simplifies subsequent relations; λ represents the stretch from the microstructural configuration to the reference.

so that their component matrices have the respective forms

$$\begin{bmatrix} \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \begin{bmatrix} \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Tensor fields that are independent of X_3 and of the form $(3.21)_1$ are termed **planar**. Note that this definition excludes $\boldsymbol{L}$, which annihilates vectors parallel to $\boldsymbol{e}$.

The constraint of plane strain does not generally render $\boldsymbol{F}^p$ and $\boldsymbol{F}^e$ planar tensors. Indeed, for a rigid-plastic material, the polar decomposition (3.6) yields $\boldsymbol{F}=(\boldsymbol{R}^e\boldsymbol{R}^p)\boldsymbol{U}^p$ with $\boldsymbol{U}^p$ the square root of $\boldsymbol{F}^\top\boldsymbol{F}$; hence $\boldsymbol{U}^p$ and $\boldsymbol{R}^e\boldsymbol{R}^p$ must be planar, but individually $\boldsymbol{R}^e$ and $\boldsymbol{R}^p$ need not be planar.

A direct consequence of (3.4) is that, if $\boldsymbol{F}^p$ is planar at some time, then $\boldsymbol{F}^p$ and (hence) $\boldsymbol{F}^e$ are planar if and only if

$$\boldsymbol{L}^p\boldsymbol{e} = \boldsymbol{L}^{p\top}\boldsymbol{e} = \boldsymbol{0} \tag{3.22}$$

(so that $\boldsymbol{L}^p$ has the form $(3.21)_2$). We use the term **strict plane strain** to describe plane strain with $\boldsymbol{F}^p$ and $\boldsymbol{F}^e$ *planar tensor fields*. Under strict plane strain, $\boldsymbol{F}^p\boldsymbol{e}=\boldsymbol{e}$ and $\boldsymbol{F}^{p\top}\boldsymbol{e}=\boldsymbol{e}$, and similarly for $\boldsymbol{F}^e$ (and $\boldsymbol{F}$); hence *referential planes perpendicular to* $\boldsymbol{e}$ *convect to planes perpendicular to* $\boldsymbol{e}$ *in the microstructural and deformed configurations.*

For single crystals one can be assured of strict plane strain provided one restricts attention to **planar slip systems**;[18] that is, slip systems α that satisfy

$$\boldsymbol{s}^\alpha\cdot\boldsymbol{e} = 0, \qquad \boldsymbol{m}^\alpha\cdot\boldsymbol{e} = 0, \qquad \boldsymbol{s}^\alpha \times \boldsymbol{m}^\alpha = \boldsymbol{e}, \tag{3.23}$$

with slips ν^α independent of X_3. (The requirement $(3.23)_3$ involves no loss in generality.)

4 Burgers vector. The geometric dislocation tensor $\boldsymbol{G}$

By $(2.13)_1$, $\operatorname{Curl}\boldsymbol{F}^p = \boldsymbol{0}$ when the plastic strain is **compatible** (the gradient of a vector field); $\operatorname{Curl}\boldsymbol{F}^p$ therefore provides a measure of the incompatibility of the plastic strain. By Stokes' theorem, for ∂S_{R} the boundary curve of a smooth surface S_{R} in the *reference body*,

$$\boldsymbol{b}_{\mathrm{R}}(\partial S_{\mathrm{R}}) \equiv \int_{\partial S_{\mathrm{R}}} \boldsymbol{F}^p d\boldsymbol{X} = \int_{S_{\mathrm{R}}} (\operatorname{Curl}\boldsymbol{F}^p)^\top \boldsymbol{n}_{\mathrm{R}}\, dA_{\mathrm{R}}. \tag{4.1}$$

For a single crystal the microscopic structure is a lattice and, since the vector $(\operatorname{Curl}\boldsymbol{F}^p)^\top\boldsymbol{n}_{\mathrm{R}}$ lies in the *lattice configuration*, one might associate

$$(\operatorname{Curl}\boldsymbol{F}^p)^\top \boldsymbol{n}_{\mathrm{R}}\, dA_{\mathrm{R}}$$

with the Burgers vector corresponding to the boundary curve of a surface-element with normal $\boldsymbol{n}_{\mathrm{R}}$, but that would be incorrect, as the surface element $\boldsymbol{n}_{\mathrm{R}}\, dA_{\mathrm{R}}$ lies in the *reference configuration* rather than in the lattice configuration. This is easily rectified. By (3.11), $\boldsymbol{n}\, dA = J^p\boldsymbol{F}^{p-\top}\boldsymbol{n}_{\mathrm{R}}\, dA_{\mathrm{R}}$ is the surface element in the lattice configuration from which $\boldsymbol{n}_{\mathrm{R}}\, dA_{\mathrm{R}}$ convects; thus, formally,

$$(\operatorname{Curl}\boldsymbol{F}^p)^\top \boldsymbol{n}_{\mathrm{R}}\, dA_{\mathrm{R}} = \frac{1}{J^p}(\operatorname{Curl}\boldsymbol{F}^p)^\top \boldsymbol{F}^{p\top}\boldsymbol{n}\, dA, \tag{4.2}$$

with $\boldsymbol{n}\, dA$ the surface element in the lattice configuration, so that

$$\frac{1}{J^p}(\boldsymbol{F}^p \operatorname{Curl}\boldsymbol{F}^p)^\top \boldsymbol{n}\, dA$$

[18] All other slip systems are ignored. There is a large literature based on this hypothesis. The resulting fully two-dimensional kinematics is important in constructing simple mathematical models, often based on two slip systems. Cf., e.g., Asaro (1983, pp. 45-46, 84-97) and the references therein, and Prantil, Jenkins and Dawson (1993). Cf. also Kalidindi and Anand (1993), who discuss plane strain allowing for a full three-dimensional collection of slip systems.

is the *local Burgers vector* corresponding to the "boundary curve" of the surface element $\boldsymbol{n}\,dA$ in the *lattice configuration.* Thus, for

$$\boldsymbol{G}^p = \frac{1}{J^p}\boldsymbol{F}^p\,\mathrm{Curl}\,\boldsymbol{F}^p, \tag{4.3}$$

$\boldsymbol{G}^{p\top}\boldsymbol{n}$ provides a measure — based on the plastic strain — of the (local) Burgers vector in the lattice configuration — per unit area in that configuration — for the plane Π with unit normal $\boldsymbol{n}$.

On the other hand, let $\bar{S}$ be a smooth surface in the *deformed body* and consider the line integral

$$\bar{\boldsymbol{b}}(\partial\bar{S}) \equiv \int_{\partial\bar{S}} \boldsymbol{F}^{e-1}d\boldsymbol{x} = \int_{\bar{S}}(\mathrm{curl}\,\boldsymbol{F}^{e-1})^{\top}\bar{\boldsymbol{n}}\,d\bar{A} \tag{4.4}$$

$(\boldsymbol{F}^{e-1} = (\boldsymbol{F}^e)^{-1})$. As before, $\mathrm{curl}\,\boldsymbol{F}^{e-1} = \boldsymbol{0}$ when $\boldsymbol{F}^e$ is compatible; $\mathrm{curl}\,\boldsymbol{F}^{e-1}$ therefore provides a measure of the local incompatibility of the structural deformation. Arguing as in the steps leading to (4.3), we may use (3.13), again formally, to conclude that

$$(\mathrm{curl}\,\boldsymbol{F}^{e-1})^{\top}\bar{\boldsymbol{n}}\,d\bar{A} = J^e(\mathrm{curl}\,\boldsymbol{F}^{e-1})^{\top}\boldsymbol{F}^{e-\top}\boldsymbol{n}\,dA.$$

Thus, by (4.5), for

$$\boldsymbol{G}^e = J^e\boldsymbol{F}^{e-1}\mathrm{curl}\,\boldsymbol{F}^{e-1},$$

$\boldsymbol{G}^{e\top}\boldsymbol{n}$ provides a measure — based on the elastic deformation — of the Burgers vector, per unit area in the lattice configuration, for the plane Π with unit normal $\boldsymbol{n}$.

$\boldsymbol{G}^{p\top}\boldsymbol{n}$ and $\boldsymbol{G}^{e\top}\boldsymbol{n}$ purportedly characterize the same Burgers vector. To reconcile this, note that, if $\bar{S}$ convects from S_{R}, then

$$\int_{\partial S_{\mathrm{R}}} \boldsymbol{F}^p d\boldsymbol{X} = \int_{\partial S_{\mathrm{R}}} \boldsymbol{F}^p\boldsymbol{F}^{-1}\boldsymbol{F}d\boldsymbol{X} = \int_{\partial\bar{S}} \boldsymbol{F}^{e-1}d\boldsymbol{x},$$

so that

$$\bar{\boldsymbol{b}}(\partial\bar{S}) = \boldsymbol{b}_{\mathrm{R}}(\partial S_{\mathrm{R}}). \tag{4.5}$$

Therefore, by (3.9),

$$\int_{S_{\mathrm{R}}}(\mathrm{Curl}\,\boldsymbol{F}^p)^{\top}\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}} = \int_{\bar{S}}(\mathrm{curl}\,\boldsymbol{F}^{e-1})^{\top}\bar{\boldsymbol{n}}\,d\bar{A} = \int_{S_{\mathrm{R}}}(J(\mathrm{curl}\,\boldsymbol{F}^{e-1})^{\top}\boldsymbol{F}^{-\top}\boldsymbol{n}_{\mathrm{R}})\,dA_{\mathrm{R}},$$

and, as $\bar{S}$ is arbitrary,

$$(\mathrm{Curl}\,\boldsymbol{F}^p)^{\top} = J(\mathrm{curl}\,\boldsymbol{F}^{e-1})^{\top}\boldsymbol{F}^{-\top}.$$

Thus, since $\boldsymbol{F} = \boldsymbol{F}^e\boldsymbol{F}^p$ and $J = J^eJ^p$, we have the

EQUIVALENCE THEOREM. *The tensor fields $\boldsymbol{G}^p$ and $\boldsymbol{G}^e$ coincide. We refer to*

$$\boldsymbol{G} = \frac{1}{J^p}\boldsymbol{F}^p\,\mathrm{Curl}\,\boldsymbol{F}^p = J^e\boldsymbol{F}^{e-1}\mathrm{curl}\,\boldsymbol{F}^{e-1} \tag{4.6}$$

as the **geometric dislocation tensor**.

Reiterating, $\boldsymbol{G}^{\top}\boldsymbol{n}$ represents the (local) **Burgers vector** in the microstructural configuration — per unit area in that configuration — for the plane Π with unit normal $\boldsymbol{n}$.[19] Here and what follows, *we refer to $\boldsymbol{G}^{\top}\boldsymbol{n}$ as the Burgers vector even when the microstructural configuration does not represent a single crystal.*

REMARK. An important consequence of the equivalence theorem is that arguments regarding $\boldsymbol{G}$ are invariant under the replacement of the field $\boldsymbol{F}^p$ by the field $\boldsymbol{F}^{e-1}$ provided operations in the reference configuration are replaced by analogous operations in the deformed configuration.

[19]Or in more physical terms, the local Burgers vector, per unit area, for those dislocation lines piercing Π.

5 Canonical decompositions of the geometric dislocation tensor

5.1 Decompositions into tensors of simple structure

Because of its tensorial nature, $\mathbf{G}$ bears some comparison to the tensors of strain and stress. An infinitesimal strain tensor may be written as a sum of simple extensions in mutually perpendicular directions, or *equivalently* as a purely volumetric strain plus simple shears on three mutually perpendicular planes. Decompositions of this type apply also to $\mathbf{G}$, but with different physical interpretation. The building blocks of such decompositions form the content of the following definitions; in these definitions attention is focused on a given material point, and $\boldsymbol{\ell}$ is a *unit vector.*

(*a*) $\mathbf{G}$ is a **pure edge-tensor** if

$$\mathbf{G} = \boldsymbol{\ell}\otimes\mathbf{g} \quad \text{with } \mathbf{g} \text{ perpendicular to } \boldsymbol{\ell}, \tag{5.1}$$

so that $\mathbf{g}$, the Burgers vector for $\boldsymbol{\ell}^{\perp}$, is parallel to the plane $\boldsymbol{\ell}^{\perp}$. In this case $\mathbf{g}$ is termed the **principal Burgers vector** and $\boldsymbol{\ell}$ is the **line direction.**

(*b*) $\mathbf{G}$ is a **pure screw-tensor** if

$$\mathbf{G} = \boldsymbol{\ell}\otimes\mathbf{h} \quad \text{with } \mathbf{h} \text{ parallel to } \boldsymbol{\ell}, \tag{5.2}$$

so that $\mathbf{G}^{\top}\boldsymbol{\ell}=\mathbf{h}$, the Burgers vector for the plane $\boldsymbol{\ell}^{\perp}$, is perpendicular to $\boldsymbol{\ell}^{\perp}$. In this case $\mathbf{h}$ is termed the **principal Burgers vector** and $\boldsymbol{\ell}$ is the **line direction.**

(*c*) $\mathbf{G}$ is an **axial edge-tensor** if

$$\mathbf{G} = \boldsymbol{\xi}\times,$$

so that, given any $\mathbf{n}$, the Burgers vector $\mathbf{G}^{\top}\mathbf{n}$ is always parallel to the plane $\mathbf{n}^{\perp}$.

(*d*) $\mathbf{G}$ is an **isotropic screw-tensor** if

$$\mathbf{G} = \varphi\mathbf{1},$$

so that, given any $\mathbf{n}$, the Burgers vector $\mathbf{G}^{\top}\mathbf{n}$ is always is always perpendicular to the plane $\mathbf{n}^{\perp}$.

As we shall see, $\mathbf{G}$ is a pure edge-tensor for plane strain and a pure screw-tensor for anti-plane shear, and in each case the line direction is normal to the cross-sectional plane of the body.

Given an axial edge-tensor $\mathbf{G}=\boldsymbol{\xi}\times$ and *any* orthogonal unit vectors $\mathbf{n}$ and $\mathbf{m}$ each orthogonal to $\boldsymbol{\xi}$ and such that $\mathbf{n}\times\mathbf{m}$ points in the direction of $\boldsymbol{\xi}$, we have the decomposition

$$\mathbf{G} = \mathbf{m}\otimes(|\boldsymbol{\xi}|\mathbf{n}) - \mathbf{n}\otimes(|\boldsymbol{\xi}|\mathbf{m})$$

of $\mathbf{G}$ into pure edge-tensors with orthogonal line directions. Similarly given an isotropic screw-tensor $\mathbf{G}=\varphi\mathbf{1}$ and an orthonormal basis $\{\boldsymbol{\ell}_1,\boldsymbol{\ell}_2,\boldsymbol{\ell}_3\}$, we have the decomposition

$$\mathbf{G} = \sum_{i=1}^{3}\boldsymbol{\ell}_i\otimes(\varphi\boldsymbol{\ell}_i).$$

of $\mathbf{G}$ into pure screws with mutually orthogonal line directions and Burgers vectors of equal magnitude. Decompositions of this type are special cases of the

FIRST DECOMPOSITION THEOREM.[20] *Given any material point, the geometric dislocation tensor* $\mathbf{G}$ *may be decomposed:*

(*i*) *into an isotropic screw-tensor plus a sum of three pure edge-tensors with respect to mutually orthogonal planes; specifically, there are a scalar* φ*, an orthonormal basis* $\{\boldsymbol{\ell}_1,\boldsymbol{\ell}_2,\boldsymbol{\ell}_3\}$*, and vectors* $\{\mathbf{g}_1,\mathbf{g}_2,\mathbf{g}_3\}$ *with* $\mathbf{g}_i$ **perpendicular** *to* $\boldsymbol{\ell}_i$ *such that*

$$\mathbf{G} = \varphi\mathbf{1} + \sum_{i=1}^{3}\boldsymbol{\ell}_i\otimes\mathbf{g}_i; \tag{5.3}$$

[20] The orthonormal basis $\{\boldsymbol{\ell}_1,\boldsymbol{\ell}_2,\boldsymbol{\ell}_3\}$ in (*i*) is generally different from that in (*ii*).

(*ii*) *into an axial edge-tensor plus a sum of three pure screw-tensors with mutually orthogonal Burgers vectors; specifically, there are a vector* $\boldsymbol{\xi}$*, an orthonormal basis* $\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}$*, and vectors* $\{\boldsymbol{h}_1, \boldsymbol{h}_2, \boldsymbol{h}_3\}$ *with* $\boldsymbol{h}_i$ **parallel** *to* $\boldsymbol{\ell}_i$ *such that*

$$\boldsymbol{G} = (\boldsymbol{\xi}\times) + \sum_{i=1}^{3} \boldsymbol{\ell}_i \otimes \boldsymbol{h}_i. \tag{5.4}$$

Proof. (*i*) Consequences of standard results are that $\boldsymbol{G}$ may be written in the form

$$\boldsymbol{G} = \varphi\mathbf{1} + \boldsymbol{G}_0, \qquad \operatorname{tr}\boldsymbol{G}_0 = 0.$$

Further, there are scalars $\{\kappa_1, \kappa_2, \kappa_3\}$ and an orthonormal basis $\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}$ such that[21]

$$\operatorname{sym}\boldsymbol{G}_0 = \operatorname{sym}(\kappa_3\mathbb{N}_{12} + \kappa_2\mathbb{N}_{31} + \kappa_1\mathbb{N}_{23}), \qquad \mathbb{N}_{ij} = \boldsymbol{\ell}_i \otimes \boldsymbol{\ell}_j,$$

and, given this decomposition, there are scalars $\{\zeta_1, \zeta_2, \zeta_3\}$ such that

$$\operatorname{skw}\boldsymbol{G}_0 = -2\operatorname{skw}(\zeta_3\mathbb{N}_{12} + \zeta_2\mathbb{N}_{31} + \zeta_1\mathbb{N}_{23}).$$

Thus, letting

$$\boldsymbol{g}_1 = (\kappa_3 - \zeta_3)\boldsymbol{\ell}_2 + (\kappa_2 + \zeta_2)\boldsymbol{\ell}_3, \qquad \boldsymbol{g}_2 = \dots, \qquad \boldsymbol{g}_3 = \dots$$

(with $\boldsymbol{g}_2$ and $\boldsymbol{g}_3$ obtained by cyclic permutation of the indices), we find that

$$\boldsymbol{G}_0 = \sum_{i=1}^{3} \boldsymbol{\ell}_i \otimes \boldsymbol{g}_i,$$

which implies (5.3), since $\boldsymbol{G}_0 = \operatorname{sym}\boldsymbol{G}_0 + \operatorname{skw}\boldsymbol{G}_0$.

(*ii*) There are an orthonormal basis $\{\boldsymbol{\ell}_1, \boldsymbol{\ell}_2, \boldsymbol{\ell}_3\}$, scalars $\{\lambda_1, \lambda_2, \lambda_3\}$, and a vector $\boldsymbol{\xi}$, the axial vector of $\operatorname{skw}\boldsymbol{G}$, such that

$$\operatorname{sym}\boldsymbol{G} = \sum_{i=1}^{3} \lambda_i \boldsymbol{\ell}_i \otimes \boldsymbol{\ell}_i, \qquad \operatorname{skw}\boldsymbol{G} = \boldsymbol{\xi}\times\,,$$

which yields (5.4) and completes the proof of the theorem.

A consequence of this proof are the following identities:

$$\operatorname{tr}\boldsymbol{G} = 3\varphi, \qquad |\,\boldsymbol{G}_0\,|^2 = \sum_{i=1}^{3} |\,\boldsymbol{g}_i\,|^2, \qquad |\operatorname{skw}\boldsymbol{G}\,|^2 = 2|\,\boldsymbol{\xi}\,|^2, \qquad |\operatorname{sym}\boldsymbol{G}\,|^2 = \sum_{i=1}^{3} |\,\boldsymbol{h}_i\,|^2. \tag{5.5}$$

5.2 Decomposition into isochoric and dilatational parts

By (3.17), for the special case of a dilatation, $\boldsymbol{G}$ is an axial edge-tensor:

$$\boldsymbol{G} = -(\nabla\lambda\,\times). \tag{5.6}$$

More generally, we have the following consequence of (4.6):

SECOND DECOMPOSITION THEOREM. *Consider the decomposition* $\boldsymbol{F}^p = \lambda^{-1}\boldsymbol{F}^p_0$, $\det\boldsymbol{F}^p_0 = 1$, *of* $\boldsymbol{F}^p$ *into isochoric and dilatational parts* (cf. (3.19)). *Then*

$$\boldsymbol{G} = \lambda\boldsymbol{G}_0 - \boldsymbol{F}^p_0\,(\nabla\lambda\,\times)\,\boldsymbol{F}^{p\top}_0 \tag{5.7}$$

with

$$\boldsymbol{G}_0 = \boldsymbol{F}^p_0\operatorname{Curl}\boldsymbol{F}^p_0$$

the geometric dislocation tensor for the isochoric part of $\boldsymbol{F}^p$.

[21] This is simply the decomposition of a deviatoric "strain tensor" into simple shears on mutually orthogonal planes. Cf., e.g., Gurtin (1972, p. 36).

6 $\boldsymbol{G}$ described relative to the reference and deformed configurations

6.1 The tensors $\boldsymbol{G}_{\mathrm{R}}$ and $\bar{\boldsymbol{G}}$

$\boldsymbol{G}$ has a referential counterpart that may be obtained by transforming the vector $\boldsymbol{G}^{\top}\boldsymbol{n}dA$ to the reference configuration by premultiplication by $\boldsymbol{F}^{p-1}$ and then converting $\boldsymbol{n}\,dA$ to the referential surface element $\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}}$ using (3.11); the result is

$$\boldsymbol{G}_{\mathrm{R}} = J^p\boldsymbol{F}^{p-1}\boldsymbol{G}\boldsymbol{F}^{p-\top} = (\mathrm{Curl}\,\boldsymbol{F}^p)\boldsymbol{F}^{p-\top}; \tag{6.1}$$

$\boldsymbol{G}_{\mathrm{R}}^{\top}\boldsymbol{n}_{\mathrm{R}}$ gives the Burgers vector transported back to — and measured per unit area in — the reference configuration, $\boldsymbol{n}_{\mathrm{R}}\,dA_{\mathrm{R}}$ being the relevant surface element. Similarly, transforming $\boldsymbol{G}^{\top}\boldsymbol{n}dA$ to the deformed configuration by premultiplication by $\boldsymbol{F}^e$ and then converting $\boldsymbol{n}\,dA$ to the deformed surface element $\bar{\boldsymbol{n}}\,d\bar{A}$ using (3.13) results in the tensor field

$$\bar{\boldsymbol{G}} = \frac{1}{J^e}\boldsymbol{F}^e\boldsymbol{G}\boldsymbol{F}^{e\top} = (\mathrm{curl}\,\boldsymbol{F}^{e-1})\boldsymbol{F}^{e\top}; \tag{6.2}$$

$\bar{\boldsymbol{G}}^{\top}\bar{\boldsymbol{n}}$ gives the Burgers vector convected to — and measured per unit area in — the deformed configuration, $\bar{\boldsymbol{n}}\,d\bar{A}$ being the relevant surface element. $\boldsymbol{G}_{\mathrm{R}}$ and $\bar{\boldsymbol{G}}$ represent the geometric dislocation tensor $\boldsymbol{G}$ referred, respectively, to the reference and deformed configurations.

6.2 Transformation of the microstructural configuration

A **homogeneous transformation of the microstructural configuration** is defined by a constant invertible tensor $\boldsymbol{M}$ together with the transformations:

$$\boldsymbol{F}^{p*} = \boldsymbol{M}\boldsymbol{F}^p, \qquad \boldsymbol{F}^{e*} = \boldsymbol{F}^e\boldsymbol{M}^{-1} \tag{6.3}$$

(so that $\boldsymbol{F}^* = \boldsymbol{F}$). Under such a transformation

$$\left.\begin{aligned} \boldsymbol{G}^* &= J^{e*}(\boldsymbol{F}^{e*})^{-1}\mathrm{curl}\left((\boldsymbol{F}^{e*})^{-1}\right) = \frac{1}{J^{p*}}\boldsymbol{F}^{p*}\,\mathrm{Curl}\,\boldsymbol{F}^{p*},\\ \boldsymbol{G}^*_{\mathrm{R}} &= (\mathrm{Curl}\,\boldsymbol{F}^{p*})(\boldsymbol{F}^{p*})^{-\top}, \quad \bar{\boldsymbol{G}}^* = \mathrm{curl}\left((\boldsymbol{F}^{e*})^{-1}\right)(\boldsymbol{F}^{e*})^{\top}.\end{aligned}\right\} \tag{6.4}$$

By $(2.13)_2$,

$$\mathrm{Curl}\,(\boldsymbol{M}\boldsymbol{F}^p) = (\mathrm{Curl}\,\boldsymbol{F}^p)\boldsymbol{M}^{\top}, \qquad \mathrm{curl}\left((\boldsymbol{F}^e\boldsymbol{M}^{-1})^{-1}\right) = (\mathrm{curl}\,\boldsymbol{F}^{e-1})\boldsymbol{M}^{\top},$$

and this yields the

TRANSFORMATION THEOREM. *Under a homogeneous transformation of the microstructural configuration the geometric dislocation tensor transforms according to*

$$\boldsymbol{G}^* = (\det\boldsymbol{M})^{-1}\boldsymbol{M}\boldsymbol{G}\boldsymbol{M}^{\top}. \tag{6.5}$$

On the other hand, $\boldsymbol{G}^*_{\mathrm{R}} = \boldsymbol{G}_{\mathrm{R}}$ and $\bar{\boldsymbol{G}}^* = \bar{\boldsymbol{G}}$, *so that the geometric dislocation tensor — when referred to the reference or deformed configuration — is invariant.*

For a *rigid-plastic material* the local relation between the lattice and the deformed configuration is a rotation $\boldsymbol{R}^e$, and the lattice as it would appear to an observer is simply the lattice as framed in the microstructural configuration rotated via $\boldsymbol{R}^e$. The tensor

$$\bar{\boldsymbol{G}} = \boldsymbol{R}^e\boldsymbol{G}\boldsymbol{R}^{e\top} = (\mathrm{curl}\,\boldsymbol{R}^{e\top})\boldsymbol{R}^{e\top} \tag{6.6}$$

therefore represents the **true Burgers vector**; that is, the Burgers vector as seen by an observer. Measurements of lattice rotations are generally made with respect to the orientation of the lattice at a particular point $\boldsymbol{x}_0$ in the deformed configuration. With this in mind, let $\boldsymbol{R}^e_0$ denote the lattice rotation at $\boldsymbol{x}_0$, so that

$$\boldsymbol{Q}^e = \boldsymbol{R}^e\boldsymbol{R}^{e\top}_0$$

represents the rotation from $\boldsymbol{x}_0$ to $\boldsymbol{x}$. Further, choose $\boldsymbol{M}=\boldsymbol{R}_0^e$ in the transformation (6.3) and write $\bar{\boldsymbol{G}}_0=\bar{\boldsymbol{G}}^*$. Then $\bar{\boldsymbol{G}}_0$ *represents the true Burgers vector as reckoned by an experimenter who measures lattice rotations with respect to* $\boldsymbol{x}_0$, and, by $(6.3)_2$,

$$\bar{\boldsymbol{G}}_0 = (\mathrm{curl}\,\boldsymbol{Q}^{e\top})\boldsymbol{Q}^{e\top}.$$

Thus, when convenient, we may, at any given time, identify the lattice configuration with the lattice at a particular point $\boldsymbol{x}_0$ in the deformed configuration. Consistent with this one replaces $\boldsymbol{R}^e$ by $\boldsymbol{Q}^e=\boldsymbol{R}^e\boldsymbol{R}_0^{e\top}$ and $\boldsymbol{F}^p$ by $\boldsymbol{R}_0^e\boldsymbol{F}^p$.

7 Rigid-plastic materials. Euler-angle representation of $\boldsymbol{G}$

In situations for which elastic strains are negligible, geometrically necessary dislocations are amenable to experimental study through the measurement of lattice rotations. Further, since lattice orientation is often characterized through the use of Euler angles, it would seem important to have at hand a simple relation for $\boldsymbol{G}$ in terms of gradients of Euler angles. This is the central objective of this section.

7.1 Representation of rotations

The discussion of rotations is greatly simplified using the exponential of a tensor $\boldsymbol{A}$ as defined by the power series

$$\exp(\boldsymbol{A}) = \sum_{k=0}^{\infty}\frac{1}{k!}\boldsymbol{A}^k, \tag{7.1}$$

a definition that renders

$$\boldsymbol{Z}(\vartheta) = \exp(\vartheta\boldsymbol{A})$$

the unique solution of the initial-value problem

$$\frac{d\boldsymbol{Z}}{d\vartheta} = \boldsymbol{A}\boldsymbol{Z}, \qquad \boldsymbol{Z}(0) = \mathbf{1}. \tag{7.2}$$

If $\boldsymbol{W}$ is a skew tensor, then $\boldsymbol{R}=\exp(\boldsymbol{W})$ is a rotation, and any such rotation $\boldsymbol{R}$ may be written in this form. In particular, given a unit vector $\mathbf{e}$ and a scalar ϑ,

$$\boldsymbol{Q}(\vartheta,\mathbf{e}) \stackrel{\text{def}}{=} \exp(\vartheta\,\mathbf{e}\times) \tag{7.3}$$

represents the rotation about $\mathbf{e}$ whose counterclockwise angle of rotation is ϑ. Fix $\mathbf{e}$ and consider (7.3) as a function $\boldsymbol{Q}(\vartheta)=\boldsymbol{Q}(\vartheta,\mathbf{e})$. Then

$$\frac{d\boldsymbol{Q}}{d\vartheta} = (\mathbf{e}\times)\,\boldsymbol{Q}, \qquad \frac{d\boldsymbol{Q}^\top}{d\vartheta} = -(\mathbf{e}\times)\,\boldsymbol{Q}^\top. \tag{7.4}$$

The first identity follows from (7.2). To establish the second, note that, since $\boldsymbol{Q}$ is a rotation about $\mathbf{e}$, $(\mathbf{e}\times)\boldsymbol{Q}^\top=\boldsymbol{Q}^\top(\mathbf{e}\times)$. Thus, since $\mathbf{e}\times$ is skew, $(7.4)_1$ implies $(7.4)_2$.

A representation of a rotation $\boldsymbol{R}$ in terms of **Euler-angles**[22] is a decomposition of $\boldsymbol{R}$ into the product of three rotations

$$\boldsymbol{R} = \boldsymbol{Q}(\vartheta_3,\boldsymbol{c}_3)\,\boldsymbol{Q}(\vartheta_2,\boldsymbol{c}_2)\,\boldsymbol{Q}(\vartheta_1,\boldsymbol{c}_1) \tag{7.5}$$

of angles ϑ_i about unit vectors $\boldsymbol{c}_i$. The standard Euler-angle representation is obtained by choosing $\boldsymbol{c}_1=\boldsymbol{c}_3=\boldsymbol{k}$ and $\boldsymbol{c}_2=\boldsymbol{i}$, with $(\boldsymbol{i},\boldsymbol{j},\boldsymbol{k})$ an orthogonal basis; in this case the angles are generally denoted by $\vartheta_3=\varphi_1$, $\vartheta_2=\psi$, $\vartheta_1=\varphi_2$, so that

$$\boldsymbol{R} = \boldsymbol{Q}(\varphi_1,\boldsymbol{k})\,\boldsymbol{Q}(\psi,\boldsymbol{i})\,\boldsymbol{Q}(\varphi_2,\boldsymbol{k}), \qquad \varphi_1,\varphi_2\in[0,2\pi), \quad \psi\in[0,\pi]. \tag{7.6}$$

Any rotation may be represented in the standard form (7.6).

[22] Cf., e.g., Synge (1960) and Kocks, Tomé and Wenk (1998) for discussions of this and other rotation-representations common in mechanics and materials science.

7.2 Euler-angle representation of G

It is most convenient to work with the geometric dislocation tensor

$$\bar{G} = R^e G R^{e\top} = (\operatorname{curl} R^{e\top}) R^{e\top}$$

(cf.(6.6)) referred to the deformed configuration.

Consider the Euler-angle decomposition[23]

$$R^e = Q_3 Q_2 Q_1, \qquad Q_i(x) = Q(\vartheta_i(x), c_i)$$

where the c_i are *constant* unit vectors (with c_1 microstructural). Before proceding with the calculation of $\bar{G}$, note that since c_1 is the axis of the initial rotation Q_1, $Q_3 Q_2 Q_1 c_1 = Q_3 Q_2 c_1$ represents c_1 convected to the deformed configuration; and, since the rotation Q_2 follows Q_1, $Q_3 Q_2 c_2 = Q_3 c_2$ represents the convected value of c_2. The unit vectors

$$\bar{c}_1 = Q_3 Q_2 c_1, \qquad \bar{c}_2 = Q_3 c_2, \qquad \bar{c}_3 = c_3$$

therefore represent the vectors c_i convected to the deformed configuration.

To calculate $\bar{G}$, note that, by (2.14), (2.16), and (7.4), for B a rotation,

$$\begin{aligned} \operatorname{curl}(Q_i^\top B^\top) &= (\operatorname{curl} B^\top) Q_i + (\operatorname{grad}\vartheta_i \times) B (c_i \times) Q_i, \\ &= (\operatorname{curl} B^\top) Q_i + (\operatorname{grad}\vartheta_i \times)\{(B c_i)\times\} B Q_i. \end{aligned} \tag{7.7}$$

Applying (7.7) with $i=1$ and $B = Q_3 Q_2$ yields

$$\operatorname{curl} R^{e\top} = \{\operatorname{curl}(Q_2^\top Q_3^\top)\} Q_1 + (\operatorname{grad}\vartheta_1 \times)\{(Q_3 Q_2 c_1)\times\} Q_3 Q_2 Q_1.$$

Two more applications of (7.7), first to $\operatorname{curl}(Q_2^\top Q_3^\top)$ and then to $\operatorname{curl}(Q_3^\top)$, leads to the expression

$$\operatorname{curl} R^{e\top} = \{(\operatorname{grad}\vartheta_3 \times)(\bar{c}_3 \times) + (\operatorname{grad}\vartheta_2 \times)(\bar{c}_2 \times) + (\operatorname{grad}\vartheta_1 \times)(\bar{c}_1 \times)\} R^e.$$

Thus, using (2.12), we are led to the following:

THEOREM. *When represented in terms of Euler angles, the geometric dislocation tensor — referred to the deformed configuration — has the form*

$$\bar{G} = \sum_{i=1}^{3} \{\bar{c}_i \otimes \operatorname{grad}\vartheta_i - (\bar{c}_i \cdot \operatorname{grad}\vartheta_i) \mathbf{1}\}. \tag{7.8}$$

7.3 Infinitesimal rotations. Formal derivation of Nye's relation

The power series expansion (7.1) of

$$R^e = \exp(\theta\times), \qquad \theta = \vartheta e,$$

yields the formal approximation

$$R^e \sim \mathbf{1} + W^e, \qquad W^e = \theta\times \tag{7.9}$$

for small rotation-angles ϑ. The tensor field W^e represents the *infinitesimal rotation* and its axial vector θ gives the **infinitesimal vector-angle** of rotation. Consistent with (7.9), we approximate the geometric dislocation tensor $G = R^{e\top} \operatorname{curl} R^{e\top}$ by the tensor field

$$G_{\text{inf}} = -\operatorname{curl} W^e = -\operatorname{curl}(\theta\times).$$

Since $\operatorname{curl}(p\times) = (\operatorname{div} p)\mathbf{1} - \operatorname{grad} p$, we are led to the following relation of Nye (1953):

$$G_{\text{inf}} = N - (\operatorname{tr} N)\mathbf{1}, \qquad N = \operatorname{grad}\theta. \tag{7.10}$$

[23] In using the standard Euler-angle decomposition for R^e to compute G, one should bear in mind that for $\psi = 0$, R^e does not uniquely determine the angles φ_1 and φ_2, a deficiency that could result in unbounded values of $\operatorname{grad}\varphi_1$ and $\operatorname{grad}\varphi_2$ near points at which $\psi = 0$.

8 When are microstructural planes undistorted?

A given microstructural plane Π — which in the case of a single crystal may or may not correspond to a crystalline plane — is represented by its unit vector $\boldsymbol{n}$. By (3.10) and (3.12), $\boldsymbol{n}$, which is *constant*, convects from a *field* $\boldsymbol{n}_{\mathrm{R}}(\boldsymbol{X})$ of unit normals in the reference configuration and to a *field* $\bar{\boldsymbol{n}}(\boldsymbol{x})$ of unit normals in the deformed configuration, where

$$\left.\begin{aligned} \lambda_{\mathrm{R}}\boldsymbol{n}_{\mathrm{R}} &= \boldsymbol{F}^{p\top}\boldsymbol{n}, \qquad & \lambda_{\mathrm{R}} &= |\boldsymbol{F}^{p\top}\boldsymbol{n}|, \\ \bar{\lambda}\bar{\boldsymbol{n}} &= \boldsymbol{F}^{e-\top}\boldsymbol{n}, \qquad & \bar{\lambda} &= |\boldsymbol{F}^{e-\top}\boldsymbol{n}|; \end{aligned}\right\} \tag{8.1}$$

and an interesting question is whether the field $\bar{\boldsymbol{n}}$, say, represents a unit normal-field for a family of smooth surfaces in the deformed configuration, either globally or locally. When this is so, the microstructural plane Π may be termed undistorted. It is the purpose of this section to show that — in sense to be made precise — *the scalar field* $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ *measures the distortion of the microstructural plane* Π.

Let Π denote a *fixed plane* in the microstructural configuration, with $\boldsymbol{n}$ its unit normal. We say that Π is **globally undistorted**[24] if the unit-normal field $\bar{\boldsymbol{n}}(\boldsymbol{x})$ to which $\boldsymbol{n}$ convects is a normal field for a family $\mathcal{F}$ of smooth surfaces in the deformed body $\bar{\mathrm{B}}$; that is, if, given any $\boldsymbol{x}$ in $\bar{\mathrm{B}}$:

(*i*) $\boldsymbol{x}$ is contained in a single surface $\bar{S}$ of the family; and

(*ii*) $\bar{\boldsymbol{n}}(\boldsymbol{x})$ is normal to $\bar{S}$ at $\boldsymbol{x}$.

Granted this, we say that Π **convects to** the family $\mathcal{F}$.

Our next theorem is a central result of the paper.

GLOBAL DISTORTION THEOREM FOR MICROSTRUCTURAL PLANES. *Choose an oriented plane* Π *in the microstructural configuration and let* $\boldsymbol{n}$ *denote its unit normal. Then a necessary and sufficient condition that* Π *be globally undistorted is that* $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ *vanish at each point of the body.*

Proof. By (4.6) and (8.1),

$$\begin{aligned} \boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} &= \frac{1}{J^p}(\boldsymbol{F}^{p\top}\boldsymbol{n})\cdot\mathrm{Curl}\,(\boldsymbol{F}^{p\top}\boldsymbol{n}) \\ &= \frac{\lambda_{\mathrm{R}}}{J^p}\boldsymbol{n}_{\mathrm{R}}\cdot[\lambda_{\mathrm{R}}\mathrm{Curl}\,\boldsymbol{n}_{\mathrm{R}} + (\nabla\lambda_{\mathrm{R}})\times\boldsymbol{n}_{\mathrm{R}}] \\ &= \frac{\lambda_{\mathrm{R}}^2}{J^p}\boldsymbol{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{n}_{\mathrm{R}}. \end{aligned} \tag{8.2}$$

Similarly,

$$\begin{aligned} \boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} &= J^e(\boldsymbol{F}^{e-\top}\boldsymbol{n})\cdot\mathrm{curl}\,(\boldsymbol{F}^{e-\top}\boldsymbol{n}) \\ &= J^e\bar{\lambda}^2\bar{\boldsymbol{n}}\cdot\mathrm{curl}\,\bar{\boldsymbol{n}}. \end{aligned} \tag{8.3}$$

We therefore have the following result, of interest in its own right.

IDENTITIES FOR $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$. *Choose a (constant) unit normal* $\boldsymbol{n}$ *in the microstructural configuration. Then*

$$\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = J^e\bar{\lambda}^2\,\bar{\boldsymbol{n}}\cdot\mathrm{curl}\,\bar{\boldsymbol{n}} = \frac{\lambda_{\mathrm{R}}^2}{J^p}\,\boldsymbol{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{n}_{\mathrm{R}}. \tag{8.4}$$

Thus a necessary and sufficient condition that $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ *vanish at a given point is that* $\bar{\boldsymbol{n}}\cdot\mathrm{curl}\,\bar{\boldsymbol{n}}=0$ (*or equivalently,* $\boldsymbol{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{n}_{\mathrm{R}}=0$).

[24]This notion could equally well have been phrased with respect to the reference configuration. Indeed, there is a family of smooth surfaces in $\bar{\mathrm{B}}$ for which $\bar{\boldsymbol{n}}$ is a normal field if and only if there is a family of smooth surfaces in $\mathrm{B_R}$ for which $\boldsymbol{n}_{\mathrm{R}}$ is a normal field.

Roughly speaking, $\bar{\boldsymbol{n}}\cdot\operatorname{curl}\bar{\boldsymbol{n}}$ represents the twist of the vector field $\bar{\boldsymbol{n}}$ about itself, and similarly for $\boldsymbol{n}_{\mathrm{R}}\cdot\operatorname{Curl}\boldsymbol{n}_{\mathrm{R}}$. Note that for a *rigid-plastic material,*

$$\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = \bar{\boldsymbol{n}}\cdot\operatorname{curl}\bar{\boldsymbol{n}}.$$

The proof of the Global Distortion Theorem follows from these identities and a classical theorem of Frobenius,[25] which asserts that a necessary and sufficient condition that $\bar{\boldsymbol{n}}(\boldsymbol{x})$ be a normal field for a family of smooth surfaces in $\bar{\mathrm{B}}$ is that $\bar{\boldsymbol{n}}\cdot\operatorname{curl}\bar{\boldsymbol{n}}=0$ everywhere in $\bar{\mathrm{B}}$.

By (5.6), $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ vanishes identically in dilatational flows; hence in such flows microstructural planes are globally undistorted.

One would generally not expect $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ to vanish everywhere, and we therefore ask whether there is a local analog of the Global Distortion Theorem appropriate to behavior in an infinitesimal neighborhood of a given point. With this in mind, choose a point $\boldsymbol{x}_0$ in the deformed configuration and consider the underlying fields as functions of the position $\boldsymbol{x}=\boldsymbol{y}(\boldsymbol{X})$ in $\bar{\mathrm{B}}$. Let Π denote a fixed plane in the microstructural configuration, with $\boldsymbol{n}$ its unit normal. We say that Π is **locally undistorted**[26] at $\boldsymbol{x}_0$ if there is a smooth, oriented surface $\bar{M}$ in $\bar{\mathrm{B}}$ through $\boldsymbol{x}_0$ such that $\bar{\boldsymbol{n}}$ and the unit normal field $\bar{\boldsymbol{m}}$ for $\bar{M}$ coincide to first-order near $\boldsymbol{x}_0$: given *any* curve $\boldsymbol{z}(\sigma)$ on $\bar{M}$ through $\boldsymbol{x}_0$ with $\boldsymbol{z}(0)=\boldsymbol{x}_0$,

$$\bar{\boldsymbol{n}}(\boldsymbol{z}(0)) = \bar{\boldsymbol{m}}(\boldsymbol{z}(0)), \qquad \left[\frac{d}{d\sigma}\bar{\boldsymbol{n}}(\boldsymbol{z}(\sigma))\right]_{\sigma=0} = \left[\frac{d}{d\sigma}\bar{\boldsymbol{m}}(\boldsymbol{z}(\sigma))\right]_{\sigma=0}. \tag{8.5}$$

LOCAL DISTORTION THEOREM FOR MICROSTRUCTURAL PLANES. *Choose an oriented plane Π in the microstructural configuration and let $\boldsymbol{n}$ denote its unit normal. Then a necessary and sufficient condition that Π be locally undistorted at a given point is that $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ vanish at that point.*

The proof of this theorem in given in the Appendix.

We say that Π is **distorted** at $\boldsymbol{x}$ if Π is not locally undistorted at $\boldsymbol{x}$; trivially, Π *is distorted at $\boldsymbol{x}$ if and only if $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}\neq 0$ at $\boldsymbol{x}$.* For this reason, we henceforth refer to the scalar field $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ as the **distortion modulus**. Finally, we list the undistorted planes for the simple forms of $\boldsymbol{G}$ discussed in Subsection 5; the results are local or global according as $\boldsymbol{G}$ has these forms at a point or at all points.

Undistorted Planes for Simple Forms of $\boldsymbol{G}$

type	$\boldsymbol{G}$	*undistorted planes*
pure edge	$\boldsymbol{n}\otimes\boldsymbol{g}$	planes parallel to $\boldsymbol{g}$, planes parallel to $\boldsymbol{n}$
pure screw	$\boldsymbol{n}\otimes\boldsymbol{h}$	planes parallel to $\boldsymbol{n}$
axial edge	$\boldsymbol{\xi}\times$	all
isotropic screw	$\varphi\mathbf{1}$	none

9 Strict plane strain

In this section we discuss the form of the geometric dislocation tensor for strict plane strain as defined in Subsection 3.6.

9.1 Identities for planar tensors

We refer to a vector field $\boldsymbol{u}$ as **planar** if $\boldsymbol{u}$ is independent of X_3 (or equivalently, x_3) and satisfies $\boldsymbol{u}\cdot\boldsymbol{e}=0$, so that $\operatorname{Curl}\boldsymbol{u}$ *is parallel to* $\boldsymbol{e}$.

IDENTITIES. *Let $\boldsymbol{T}$ be a planar tensor field. Then*

$$\operatorname{Curl}\boldsymbol{T} = \boldsymbol{e}\otimes\boldsymbol{q}, \qquad \boldsymbol{q} = (\operatorname{Curl}\boldsymbol{T})^{\top}\boldsymbol{e}, \tag{9.1}$$

[25] Cf. e.g., Choquet-Bruhat and DeWitte-Morette (1977), p. 235.

[26] This notion could equally well have been phrased relative to the reference configuration using the field $\boldsymbol{n}_{\mathrm{R}}$.

with $\boldsymbol{q}$ a planar vector field. Moreover,

$$\boldsymbol{T}(\boldsymbol{e}\times) = \det\boldsymbol{T}\,(\boldsymbol{e}\times)\boldsymbol{T}^{-\top}. \tag{9.2}$$

Proof. To verify (9.1), note that, for $\boldsymbol{c}$ a constant vector, $\boldsymbol{T}^\top\boldsymbol{c}=\boldsymbol{p}+c_3\boldsymbol{e}$ with $\boldsymbol{p}$ planar; thus, since $\operatorname{Curl}\boldsymbol{p}$ is parallel to $\boldsymbol{e}$,

$$\mathbb{P}(\boldsymbol{e})(\operatorname{Curl}\boldsymbol{T})\boldsymbol{c} = \mathbb{P}(\boldsymbol{e})\operatorname{Curl}(\boldsymbol{T}^\top\boldsymbol{c}) = \mathbb{P}(\boldsymbol{e})\operatorname{Curl}\boldsymbol{p} = \boldsymbol{0}.$$

But $\boldsymbol{c}$ is arbitrary, thus $\mathbb{P}(\boldsymbol{e})\operatorname{Curl}\boldsymbol{T}=\boldsymbol{0}$ and, since $\mathbb{P}(\boldsymbol{e})=\boldsymbol{1}-\boldsymbol{e}\otimes\boldsymbol{e}$,

$$\operatorname{Curl}\boldsymbol{T} = \boldsymbol{e}\otimes(\operatorname{Curl}\boldsymbol{T})^\top\boldsymbol{e} = \boldsymbol{e}\otimes\boldsymbol{q}. \tag{9.3}$$

Further,

$$\boldsymbol{q}\cdot\boldsymbol{e} = \boldsymbol{e}\cdot(\operatorname{Curl}\boldsymbol{T})\boldsymbol{e} = \boldsymbol{e}\cdot\operatorname{Curl}(\boldsymbol{T}^\top\boldsymbol{e}) = \boldsymbol{e}\cdot\operatorname{Curl}\boldsymbol{e} = 0$$

and $\boldsymbol{q}$ is planar. This proves the first assertion. Since $\boldsymbol{T}$ is planar, the second, (9.2), follows from (2.16):

$$\boldsymbol{T}(\boldsymbol{e}\times) = \det\boldsymbol{T}\,\{(\boldsymbol{T}^{-\top}\boldsymbol{e})\times\}\boldsymbol{T}^{-\top} = \det\boldsymbol{T}\,(\boldsymbol{e}\times)\boldsymbol{T}^{-\top}.$$

9.2 Principal Burgers vector $\boldsymbol{g}$

Under strict plane strain the tensor $\boldsymbol{G}$ simplifies considerably. By (9.1),

$$\boldsymbol{G} = \frac{1}{J^p}\boldsymbol{F}^p\operatorname{Curl}\boldsymbol{F}^p = \frac{1}{J^p}(\boldsymbol{F}^p\boldsymbol{e})\otimes(\operatorname{Curl}\boldsymbol{F}^p)^\top\boldsymbol{e} = \boldsymbol{e}\otimes(\frac{1}{J^p}\operatorname{Curl}\boldsymbol{F}^p)^\top\boldsymbol{e},$$

or equivalently,

$$\boldsymbol{G} = J^e\boldsymbol{F}^{e-1}\operatorname{curl}\boldsymbol{F}^{e-1} = \boldsymbol{e}\otimes(J^e\operatorname{curl}\boldsymbol{F}^{e-1})^\top\boldsymbol{e}.$$

We therefore have the following:

THEOREM. *Under strict plane strain the geometric dislocation tensor is a pure edge-tensor*

$$\boldsymbol{G} = \boldsymbol{e}\otimes\boldsymbol{g} \tag{9.4}$$

with principal Burgers vector $\boldsymbol{g}$ planar and of the form

$$\boldsymbol{g} = J^e(\operatorname{curl}\boldsymbol{F}^{e-1})^\top\boldsymbol{e} = \frac{1}{J^p}(\operatorname{Curl}\boldsymbol{F}^p)^\top\boldsymbol{e}. \tag{9.5}$$

Thus $\boldsymbol{g}$ represents the local Burgers vector in the microstructural configuration — per unit area in that configuration — for cross-sectional surface elements.

The distortion modulus now has the simple form

$$\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = (\boldsymbol{g}\cdot\boldsymbol{n})(\boldsymbol{e}\cdot\boldsymbol{n}); \tag{9.6}$$

thus, in view of the results of Section 8, we have the following:

THEOREM. *Under strict plane strain the distortion modulus $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n}$ vanishes on any microstructral plane Π parallel to $\boldsymbol{e}$; all such planes Π are therefore globally undistorted. Thus for a single crystal any slip system with slip plane parallel to $\boldsymbol{e}$ is globally undistorted. Finally, a microstructural plane Π not parallel to $\boldsymbol{e}$ is locally undistorted at a point if and only if $\boldsymbol{g}$ is parallel to Π.*

In view of (6.1) and (6.2), the geometric dislocation tensor is given by

$$\boldsymbol{G}_{\mathrm{R}} = \boldsymbol{e}\otimes\boldsymbol{g}_{\mathrm{R}}, \qquad \boldsymbol{g}_{\mathrm{R}} = J^p\boldsymbol{F}^{p-1}\boldsymbol{g} \tag{9.7}$$

when referred to the reference configuration, and by

$$\bar{\boldsymbol{G}} = \boldsymbol{e}\otimes\bar{\boldsymbol{g}}, \qquad \bar{\boldsymbol{g}} = \frac{1}{J^e}\boldsymbol{F}^e\boldsymbol{g}, \tag{9.8}$$

when referred to the deformed configuration.

The rotation and stretch tensors defined by the polar decomposition (3.6) of $\boldsymbol{F}^e$ are planar tensor fields; the lattice rotation $\boldsymbol{R}^e$ may therefore be expressed in the form

$$\boldsymbol{R}^e = \boldsymbol{R}^e(\vartheta^e), \tag{9.9}$$

with ϑ^e an angle that measures the lattice rotation in a counterclockwise direction about $\boldsymbol{e}$. Applying the identities (2.14) and $(7.4)_3$ to $\operatorname{Curl}\boldsymbol{F}^{e-1}$ with $\boldsymbol{F}^e = \boldsymbol{V}^e\boldsymbol{R}^e$,

$$\operatorname{curl}\boldsymbol{F}^{e-1} = (\operatorname{curl}\boldsymbol{V}^{e-1})\boldsymbol{R}^e + (\operatorname{grad}\vartheta^e\times)(\frac{d\boldsymbol{R}^{e\top}}{d\vartheta^e}\boldsymbol{V}^{e-1})^\top = (\operatorname{curl}\boldsymbol{V}^{e-1})\boldsymbol{R}^e - (\operatorname{grad}\vartheta^e\times)[(\boldsymbol{e}\times)\boldsymbol{F}^{e-1}]^\top,$$

so that,

$$\boldsymbol{g} = J^e\{\boldsymbol{R}^{e\top}(\operatorname{curl}\boldsymbol{V}^{e-1})^\top\boldsymbol{e} - (\boldsymbol{e}\times)\boldsymbol{F}^{e-1}(\boldsymbol{e}\times\operatorname{grad}\vartheta^e)\},$$

Thus, by (9.2) with $\boldsymbol{T} = \boldsymbol{F}^{e-1}$,

$$\boldsymbol{g} = J^e\boldsymbol{R}^{e\top}(\operatorname{curl}\boldsymbol{V}^{e-1})^\top\boldsymbol{e} - (\boldsymbol{e}\times)(\boldsymbol{e}\times)\boldsymbol{F}^{e-1}\operatorname{grad}\vartheta^e,$$

Further, $\boldsymbol{F}^{e-1}\operatorname{grad}\vartheta^e$ is planar and, for $\boldsymbol{u}$ planar, $(\boldsymbol{e}\times)(\boldsymbol{e}\times)\boldsymbol{u} = -\boldsymbol{u}$; thus

$$\boldsymbol{g} = J^e\,\boldsymbol{R}^{e\top}(\operatorname{curl}\boldsymbol{V}^{e-1})^\top\boldsymbol{e} + \boldsymbol{F}^{e\top}\operatorname{grad}\vartheta^e. \tag{9.10}$$

If we define the elastic left-strain $\boldsymbol{B}^e$

$$\boldsymbol{B}^e = \boldsymbol{F}^e\boldsymbol{F}^{e\top} = (\boldsymbol{V}^e)^2,$$

then, by (9.7) and (9.8), we have the following relations for the principal Burger vector referred to the deformed configuration:

$$\bar{\boldsymbol{g}} = \boldsymbol{V}^e(\operatorname{curl}\boldsymbol{V}^{e-1})^\top\boldsymbol{e} + \frac{1}{J^e}\boldsymbol{B}^e\operatorname{grad}\vartheta^e,$$

9.3 Rigid-plastic materials

9.3.1 General results

By (9.8),

$$\bar{\boldsymbol{g}} = \boldsymbol{R}^e\boldsymbol{g} \tag{9.11}$$

represents the **true Burgers vector**; that is, the Burgers vector for cross-sectional planes as would be observed by an experimenter (cf. the Remark containing (6.6)).

THEOREM. *The principal Burgers vector corresponding to a rigid-plastic material undergoing strict plane strain is given by*

$$\left.\begin{aligned}\boldsymbol{g} &= \boldsymbol{R}^{e\top}\operatorname{grad}\vartheta^e,\\ \boldsymbol{g} &= \boldsymbol{F}^{p-\top}\nabla\vartheta^e,\end{aligned}\right\} \tag{9.12}$$

Moreover, the true Burgers vector has the simple form

$$\bar{\boldsymbol{g}} = \operatorname{grad}\vartheta^e \tag{9.13}$$

and is hence normal to surfaces[27] $\vartheta^e = constant$ *in the deformed configuration.*

Proof. For a rigid-plastic material, $\boldsymbol{F}^e = \boldsymbol{R}^e$, $\operatorname{curl}\boldsymbol{V}^{e-1} = \boldsymbol{0}$, and $J^e = 1$; thus (9.10) reduces to $(9.12)_1$ and (9.13) follows. Further, $\boldsymbol{R}^{e\top}\operatorname{grad}\vartheta^e = \boldsymbol{F}^{p-\top}\nabla\vartheta^e$, since $\boldsymbol{F} = \boldsymbol{R}^e\boldsymbol{F}^p$ and $\boldsymbol{F}^\top\operatorname{grad}\vartheta^e = \nabla\vartheta^e$, and this yields

[27] Actually curves in the (1,2)-plane. Experiments on the uniaxial compression of single crystals (cf., e.g., Schwartz et. al. (1999)) exhibit regions of nearly constant lattice orientation separated by thin layers. The relation (9.13) shows that — granted strict plane strain — such layers are necessarily accompanied by geometrically necesssary dislocations and, when sufficiently thin, should have Burgers vector approximately normal to the layer.

$(9.12)_2$.

By (9.7), for $\boldsymbol{C}^p = \boldsymbol{F}^{p\top}\boldsymbol{F}^p$ the plastic right-strain,

$$g_{\mathrm{R}} = J^p \boldsymbol{C}^{p-1} \nabla \vartheta^e. \tag{9.14}$$

In many situations of interest the structural strains are small in the sense that $\boldsymbol{V}^e \approx \mathbf{1}$, so that, formally,

$$\boldsymbol{V}^{e-1} \approx \mathbf{1}, \qquad \operatorname{curl} \boldsymbol{V}^{e-1} \approx \mathbf{0}. \tag{9.15}$$

In this case the foregoing relations hold to within the same approximation.

9.3.2 Single-crystals with planar slip systems

Such single crystals have all slip systems α consistent with (3.23). Since the material is rigid-plastic, the deformed slip directions and the deformed slip-plane normals are given by

$$\bar{\boldsymbol{s}}^\alpha = \boldsymbol{R}^e \boldsymbol{s}^\alpha, \qquad \bar{\boldsymbol{m}}^\alpha = \boldsymbol{R}^e \boldsymbol{m}^\alpha, \tag{9.16}$$

and satisfy

$$\bar{\boldsymbol{s}}^\alpha \cdot \boldsymbol{e} = 0, \qquad \bar{\boldsymbol{m}}^\alpha \cdot \boldsymbol{e} = 0, \qquad \bar{\boldsymbol{m}}^\alpha \times \boldsymbol{e} = \bar{\boldsymbol{s}}. \tag{9.17}$$

THEOREM. *Let Π denote the α-th slip plane and $\Pi^\perp$ the plane perpendicular to the α-th slip direction, so that both Π and $\Pi^\perp$ are undistorted. Let $\mathcal{F}$ and $\mathcal{F}^\perp$ denote the families of smooth surfaces to which Π and $\Pi^\perp$ convect. Then the surfaces of $\mathcal{F}$ are orthogonal to the surfaces of $\mathcal{F}^\perp$, and*

$$\boldsymbol{K} = (\bar{\boldsymbol{s}}^\alpha \cdot \operatorname{grad} \vartheta^e)\, (\bar{\boldsymbol{s}}^\alpha \otimes \bar{\boldsymbol{s}}^\alpha) \tag{9.18}$$

is the curvature field for the surfaces of $\mathcal{F}$, while

$$\boldsymbol{K}^\perp = -(\bar{\boldsymbol{m}}^\alpha \cdot \operatorname{grad} \vartheta^e)\, (\bar{\boldsymbol{m}}^\alpha \otimes \bar{\boldsymbol{m}}^\alpha) \tag{9.19}$$

is the curvature field for the surfaces of $\mathcal{F}^\perp$.

Since the slip system α is fixed, we suppress the superscript α. The first sentence in the theorem is a consequence of the theorem following (9.5). By (9.16), $\bar{\boldsymbol{m}}$ and $\bar{\boldsymbol{s}}$ are unit-normal fields for the families $\mathcal{F}$ and $\mathcal{F}^\perp$; thus, since $\bar{\boldsymbol{s}} \cdot \bar{\boldsymbol{m}} = 0$, these families are orthogonal. Next, by $(7.4)_1$ and (9.9),

$$\operatorname{grad} \bar{\boldsymbol{s}} = (\frac{d\boldsymbol{R}^e}{d\vartheta^e} \boldsymbol{s}) \otimes \operatorname{grad} \vartheta^e = (\frac{d\boldsymbol{R}^e}{d\vartheta^e} \boldsymbol{R}^{e\top} \bar{\boldsymbol{s}}) \otimes \operatorname{grad} \vartheta^e = (\boldsymbol{e} \times \bar{\boldsymbol{s}}) \otimes \operatorname{grad} \vartheta^e.$$

Moreover, the same identity holds with $\boldsymbol{s}$ and $\bar{\boldsymbol{s}}$ replaced by $\boldsymbol{m}$ and $\bar{\boldsymbol{m}}$. Thus, in view of $(9.17)_3$,

$$\operatorname{grad} \bar{\boldsymbol{s}} = \bar{\boldsymbol{m}} \otimes \operatorname{grad} \vartheta^e, \qquad \operatorname{grad} \bar{\boldsymbol{m}} = -\bar{\boldsymbol{s}} \otimes \operatorname{grad} \vartheta^e. \tag{9.20}$$

The curvature field $\boldsymbol{K}$ for the family $\mathcal{F}$ is given by

$$\boldsymbol{K} = -(\operatorname{grad} \bar{\boldsymbol{m}})\, \mathbb{P}(\bar{\boldsymbol{m}}) = (\bar{\boldsymbol{s}} \otimes \operatorname{grad} \vartheta^e)\, \mathbb{P}(\bar{\boldsymbol{m}}).$$

Further (9.17) yields $\mathbb{P}(\bar{\boldsymbol{m}})\, \bar{\boldsymbol{s}} = \bar{\boldsymbol{s}}$, and, since ϑ^e is independent of x_3,

$$\mathbb{P}(\bar{\boldsymbol{m}}) \operatorname{grad} \vartheta^e = (\bar{\boldsymbol{s}} \cdot \operatorname{grad} \vartheta^e)\, \bar{\boldsymbol{s}}.$$

Thus (9.18) is satisfied; (9.19) follows similarly using $(9.20)_1$. This completes the proof.

REMARK. Under strict plane strain the underlying fields may be considered as functions of their position (x_1, x_2) in the cross-sectional plane $\mathcal{P}$. Moreover, for the special system under discussion, $\bar{\boldsymbol{s}}^\alpha$ and $\bar{\boldsymbol{m}}^\alpha$ lie in $\mathcal{P}$ and the family $\mathcal{F}$ of deformed slip planes for α may be identified with the family of smooth curves in $\mathcal{P}$ tangent to the field $\bar{\boldsymbol{s}}^\alpha$. By (9.13) and (9.18), $\bar{\boldsymbol{s}}^\alpha \cdot \operatorname{grad} \vartheta^e = \bar{\boldsymbol{s}}^\alpha \cdot \bar{\boldsymbol{g}}$ represents a curvature field for this family of curves. Similarly, $\bar{\boldsymbol{m}}^\alpha \cdot \operatorname{grad} \vartheta^e = \bar{\boldsymbol{m}}^\alpha \cdot \bar{\boldsymbol{g}}$ represents a curvature field for the family of smooth curves tangent to $\bar{\boldsymbol{m}}^\alpha$.

10 Strict anti-plane shear

Under **anti-plane shear** the deformation $\boldsymbol{x}=\boldsymbol{y}(\boldsymbol{X})$ is given by

$$x_1 = X_1, \qquad x_2 = X_2, \qquad x_3 = X_3 + u(x_1, x_2), \tag{10.1}$$

with u the displacement in the direction $\boldsymbol{e}\equiv\boldsymbol{e}_3$, and results in a deformation gradient $\boldsymbol{F}$ of the form

$$\boldsymbol{F} = \mathbf{1} + \boldsymbol{e}\otimes\boldsymbol{\gamma}, \qquad \boldsymbol{\gamma}\cdot\boldsymbol{e} = 0,$$

with $\boldsymbol{\gamma}$ independent of X_3, and with $\boldsymbol{\gamma}=\nabla u$. We require, in addition, that the anti-plane shear be **strict** in the sense that

$$\boldsymbol{F}^p = \mathbf{1} + \boldsymbol{e}\otimes\boldsymbol{\gamma}^p, \qquad \boldsymbol{F}^e = \mathbf{1} + \boldsymbol{e}\otimes\boldsymbol{\gamma}^e,$$

with $\boldsymbol{\gamma}^p$ and $\boldsymbol{\gamma}^e$ planar vectors.[28] Then

$$J^e = 1, \quad J^p = 1,$$

and, in addition, the decomposition $\boldsymbol{F}=\boldsymbol{F}^e\boldsymbol{F}^p$ yields

$$\boldsymbol{\gamma} = \boldsymbol{\gamma}^e + \boldsymbol{\gamma}^p.$$

Since $\boldsymbol{\gamma}=\nabla u$, $\operatorname{curl}\boldsymbol{\gamma}=\mathbf{0}$; thus

$$\operatorname{curl}\boldsymbol{\gamma}^p = -\operatorname{curl}\boldsymbol{\gamma}^e.$$

(By (10.1) and the fact that the underlying fields are independent of X_3, the operators "curl" and "Curl" are here interchangeable.)

Next, by $(2.13)_5$,

$$\operatorname{curl}\boldsymbol{F}^p = (\operatorname{curl}\boldsymbol{\gamma}^p)\otimes\boldsymbol{e}.$$

Moreover, since $\boldsymbol{\gamma}^p$ is planar,

$$\operatorname{curl}\boldsymbol{\gamma}^p \ \text{ and } \ \operatorname{curl}\boldsymbol{\gamma}^e \ \text{ are parallel to } \ \boldsymbol{e};$$

thus

$$\operatorname{curl}\boldsymbol{F}^p = \boldsymbol{e}\otimes\operatorname{curl}\boldsymbol{\gamma}^p$$

with $\boldsymbol{\gamma}^p\cdot\operatorname{curl}\boldsymbol{\gamma}^p=0$. Thus, since $\boldsymbol{G}=\boldsymbol{F}^p\operatorname{curl}\boldsymbol{F}^p$, we have the following:

THEOREM. *Under strict anti-plane shear the geometric dislocation tensor is a pure screw-tensor*

$$\boldsymbol{G} = \boldsymbol{e}\otimes\boldsymbol{h} \tag{10.2}$$

with (planar) principal Burgers vector

$$\boldsymbol{h} = \operatorname{curl}\boldsymbol{\gamma}^p = -\operatorname{curl}\boldsymbol{\gamma}^e. \tag{10.3}$$

Microstructural planes perpendicular to $\boldsymbol{e}$ *are therefore distorted at any point at which* $\operatorname{curl}\boldsymbol{\gamma}^p\neq\mathbf{0}$.

11 Transport of geometrically necessary dislocations

11.1 Dislocation densities. Balance law for dislocations

We show here that *kinematics alone* yields a balance law for the transport of geometrically necessary dislocations.

Within a continuum theory edge and screw dislocations are characterized by the pure edge and screw tensors (5.1) and (5.2) and hence by dyads of the form

$$\boldsymbol{\ell}\otimes\boldsymbol{b} = \begin{cases} \boldsymbol{\ell}\perp\boldsymbol{b} & \text{edge} \\ \boldsymbol{\ell}=\boldsymbol{b} & \text{screw} \end{cases} \tag{11.1}$$

[28]The notion of strict anti-plane shear is not relevant to rigid-plastic materials, as it renders $\boldsymbol{F}^e\equiv\mathbf{1}$.

with $\boldsymbol{\ell}$ and $\boldsymbol{b}$ microstructural *unit vectors*.[29] We refer to each such pair $d=(\boldsymbol{\ell},\boldsymbol{b})$ as a **dislocation dyad** with **Burgers direction** $\boldsymbol{b}$ and **line direction** $\boldsymbol{\ell}$. The scalar field

$$\rho = \rho(\boldsymbol{\ell},\boldsymbol{b}) \stackrel{\text{def}}{=} \boldsymbol{\ell}\cdot\boldsymbol{G}\boldsymbol{b} = (\boldsymbol{\ell}\otimes\boldsymbol{b})\cdot\boldsymbol{G} \tag{11.2}$$

then represents the tensor $\boldsymbol{G}$ *resolved* on the dislocation system d. We refer to $\rho(\boldsymbol{\ell},\boldsymbol{\ell})$ as a **screw density**, to $\rho(\boldsymbol{\ell},\boldsymbol{b})$ — with $\boldsymbol{b}$ *perpendicular to* $\boldsymbol{\ell}$ — as an **edge density**. Note that these densities are in units of length per unit area and are *signed.*

The vector fields

$$\boldsymbol{\ell}_{\mathrm{R}} = \boldsymbol{F}^{p\top}\boldsymbol{\ell}, \qquad \boldsymbol{b}_{\mathrm{R}} = \boldsymbol{F}^{p\top}\boldsymbol{b}$$

represent $\boldsymbol{\ell}$ and $\boldsymbol{b}$ transported back to the reference as normals, although not as unit normals. Since

$$(\mathrm{Curl}\,\boldsymbol{F}^p)\boldsymbol{b} = \mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}}, \qquad (\mathrm{Curl}\,\boldsymbol{F}^p)\boldsymbol{\ell} = \mathrm{Curl}\,\boldsymbol{\ell}_{\mathrm{R}}, \tag{11.3}$$

if $J^p=1$, then (4.6) leads to the simple expression $\rho=\boldsymbol{\ell}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}}$; hence

$$\dot\rho = \dot{\boldsymbol{\ell}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}} + \boldsymbol{\ell}_{\mathrm{R}}\cdot\mathrm{Curl}\,\dot{\boldsymbol{b}}_{\mathrm{R}} = \dot{\boldsymbol{\ell}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}} + \dot{\boldsymbol{b}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{\ell}_{\mathrm{R}} - \mathrm{Div}\,(\boldsymbol{\ell}_{\mathrm{R}}\times\dot{\boldsymbol{b}}_{\mathrm{R}}).$$

By (3.4), $\dot{\boldsymbol{\ell}}_{\mathrm{R}}=\boldsymbol{F}^{p\top}\boldsymbol{L}^{p\top}\boldsymbol{\ell}$ and $\dot{\boldsymbol{b}}_{\mathrm{R}}=\boldsymbol{F}^{p\top}\boldsymbol{L}^{p\top}\boldsymbol{b}$, so that, in view of (11.3),

$$\dot{\boldsymbol{\ell}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}} + \dot{\boldsymbol{b}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{\ell}_{\mathrm{R}} = \boldsymbol{\ell}\cdot\boldsymbol{L}^p\boldsymbol{G}\boldsymbol{b} + \boldsymbol{b}\cdot\boldsymbol{L}^p\boldsymbol{G}\boldsymbol{\ell}.$$

Further, we may use (2.16) to conclude that $(\boldsymbol{F}^{p\top}\boldsymbol{\ell})\times = \boldsymbol{F}^{p-1}(\boldsymbol{\ell}\times)\boldsymbol{F}^{p-\top}$, and hence that

$$\boldsymbol{\ell}_{\mathrm{R}}\times\dot{\boldsymbol{b}}_{\mathrm{R}} = \{(\boldsymbol{F}^{p\top}\boldsymbol{\ell})\times\}\boldsymbol{F}^{p\top}\boldsymbol{L}^{p\top}\boldsymbol{b} = \boldsymbol{F}^{p-1}(\boldsymbol{\ell}\times)\boldsymbol{L}^{p\top}\boldsymbol{b}.$$

We therefore have the[30]

BALANCE LAW FOR DISLOCATIONS. *Granted $J^p=1$, the dislocation density $\rho=\rho(\boldsymbol{\ell},\boldsymbol{b})$ has the simple form*

$$\rho = \boldsymbol{\ell}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}} \tag{11.4}$$

and evolves according to

$$\dot\rho = -\mathrm{Div}\,\boldsymbol{q}_{\mathrm{R}} + \sigma_{\mathrm{R}} \tag{11.5}$$

with $\boldsymbol{q}_{\mathrm{R}}=\boldsymbol{q}_{\mathrm{R}}(\boldsymbol{\ell},\boldsymbol{b})$ the **dislocation flux** *and $\sigma_{\mathrm{R}}=\sigma_{\mathrm{R}}(\boldsymbol{\ell},\boldsymbol{b})$ the* **dislocation supply** *defined by*

$$\left.\begin{aligned} \boldsymbol{q}_{\mathrm{R}} &= \boldsymbol{F}^{p-1}(\boldsymbol{\ell}\times(\boldsymbol{L}^{p\top}\boldsymbol{b})),\\ \sigma_{\mathrm{R}} &= 2\,(\mathrm{sym}\,\boldsymbol{\ell}\otimes\boldsymbol{b})\cdot(\boldsymbol{L}^p\boldsymbol{G}).\end{aligned}\right\} \tag{11.6}$$

As is clear from the proof, the flux and supply may be written alternatively as

$$\boldsymbol{q}_{\mathrm{R}} = \boldsymbol{\ell}_{\mathrm{R}}\times\dot{\boldsymbol{b}}_{\mathrm{R}}, \qquad \sigma_{\mathrm{R}} = \dot{\boldsymbol{\ell}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{b}_{\mathrm{R}} + \dot{\boldsymbol{b}}_{\mathrm{R}}\cdot\mathrm{Curl}\,\boldsymbol{\ell}_{\mathrm{R}}.$$

Further, for a single crystal, we may use (3.16) and (4.6) to conclude that

$$\boldsymbol{q}_{\mathrm{R}} = \sum_{\alpha=1}^{A}\nu^\alpha(\boldsymbol{b}\cdot\boldsymbol{s}^\alpha)\,\boldsymbol{F}^{p-1}(\boldsymbol{\ell}\times\boldsymbol{m}^\alpha), \qquad \sigma_{\mathrm{R}} = 2\,(\mathrm{sym}\,\boldsymbol{\ell}\otimes\boldsymbol{b})\cdot\sum_{\alpha=1}^{A}\nu^\alpha(\mathbb{S}^\alpha\boldsymbol{G}).$$

Thus slip systems α with $\boldsymbol{s}^\alpha\cdot\boldsymbol{\ell}=0$ do not contribute to temporal changes in the screw density $\rho(\boldsymbol{\ell},\boldsymbol{\ell})$; in particular, there is no contribution to changes in $\rho(\boldsymbol{m}^\beta,\boldsymbol{m}^\beta)$ from slip on β.

[29] For crystalline materials there are natural families of such dyads associated with the underlying slip systems (Sun et. al. 1998, 2000). For example, for the {111}<110> slip systems in fcc crystals a canonical set of dyads consists of twelve pure screw directions with line directions in the <110> directions and 24 pure edge directions whose line directions lie in <112> directions and whose Burgers vectors lie along <110>. But it would also seem that the screw dyads corresponding to the slip plane normals are important, as the corresponding screw densities are the distortion moduli for the slip planes.

[30] For a *non-isochoric* plastic strain $\boldsymbol{F}^p=\lambda^{-1}\boldsymbol{F}^p_0$, $\det\boldsymbol{F}^p_0=1$, the relation (5.7) yields $\rho=\lambda\rho_0-\boldsymbol{\ell}_{\mathrm{R}}\cdot(\nabla\lambda\times\boldsymbol{b}_{\mathrm{R}})$ with $\rho_0=\boldsymbol{\ell}\cdot\boldsymbol{G}_0\boldsymbol{b}$ and $\boldsymbol{G}_0=\boldsymbol{F}^p_0\,\mathrm{Curl}\,\boldsymbol{F}^p_0$.

11.2 Properties of the dislocation flux

The dislocation flux has several interesting properties. Firstly, the **microstructural flux**

$$\boldsymbol{q}(\boldsymbol{\ell},\boldsymbol{b}) \stackrel{\text{def}}{=} \boldsymbol{F}^p \boldsymbol{q}_{\mathrm{R}}(\boldsymbol{\ell},\boldsymbol{b}) = (\boldsymbol{\ell}\times)\boldsymbol{L}^{p\top}\boldsymbol{b},$$

which is $\boldsymbol{q}_{\mathrm{R}}$ convected to the microstructural configuration, lies in the plane $\boldsymbol{\ell}^{\perp}$. Moreover, plastic flow is always asociated with a flux of dislocations — that is, $\boldsymbol{L}^p \neq \boldsymbol{0}$ if and only if $\boldsymbol{q}_{\mathrm{R}}(\boldsymbol{\ell},\boldsymbol{b}) \neq \boldsymbol{0}$ for some choice of $\boldsymbol{\ell}$ and $\boldsymbol{b}$ — and this is true even when $\boldsymbol{G} \equiv \boldsymbol{0}$, but in this case $\varrho \equiv 0$, $\sigma_{\mathrm{R}} \equiv 0$, and the flow is **equilibrated**:

$$\operatorname{Div} \boldsymbol{q}_{\mathrm{R}} = 0.$$

Further, the dislocation fluxes determine $\boldsymbol{L}^p$: for $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ an arbitrarily chosen orthonormal basis and any choice of i and j, $i \neq j$,

$$\boldsymbol{e}_i \cdot \boldsymbol{L}^p \boldsymbol{e}_j = (\boldsymbol{e}_i \times \boldsymbol{e}_j) \cdot \boldsymbol{q}(\boldsymbol{e}_i, \boldsymbol{e}_i), \qquad \boldsymbol{e}_i \cdot \boldsymbol{L}^p \boldsymbol{e}_i = (\boldsymbol{e}_j \times \boldsymbol{e}_i) \cdot \boldsymbol{q}(\boldsymbol{e}_j, \boldsymbol{e}_i);$$

the off-diagonal components of $\boldsymbol{L}^p$ are therefore determined by the screw-density fluxes $\boldsymbol{q}(\boldsymbol{e}_i, \boldsymbol{e}_i)$, the diagonal components by the edge-density fluxes $\boldsymbol{q}(\boldsymbol{e}_i, \boldsymbol{e}_j)$.

Consider strict plane strain and strict anti-plane shear, and for each let $\boldsymbol{e}$ denote the out-of-plane normal. In both cases the supply vanishes identically. For strict plane strain with $\boldsymbol{b}$ planar, $\varrho(\boldsymbol{b},\boldsymbol{b})$ vanishes and $\boldsymbol{q}_{\mathrm{R}}(\boldsymbol{b},\boldsymbol{b})$ is equilibrated and parallel to $\boldsymbol{e}$, while both $\varrho(\boldsymbol{e},\boldsymbol{e})$ and $\boldsymbol{q}_{\mathrm{R}}(\boldsymbol{e},\boldsymbol{e})$ vanish. The edge densities of interest, namely $\varrho(\boldsymbol{e},\boldsymbol{b})$ with $\boldsymbol{b}$ planar, are associated with a planar lattice flux $\boldsymbol{q}$ given by $\boldsymbol{L}^{p\top}\boldsymbol{b}$ rotated about $\boldsymbol{e}$ through $\frac{\pi}{2}$. For strict anti-plane shear $\boldsymbol{L}^p$ has the form $\boldsymbol{e}\otimes\boldsymbol{\nu}$ with $\boldsymbol{\nu}$ planar and the density of interest, $\varrho(\boldsymbol{e},\boldsymbol{e})$, is associated with the lattice flux $\boldsymbol{q} = \boldsymbol{e}\times\boldsymbol{\nu}$, which is planar.

The microstructural flux $\boldsymbol{q}$ corresponding to $\boldsymbol{G}$ resolved on the dislocation system $\mathcal{d} = (\boldsymbol{\ell},\boldsymbol{b})$ was deduced simply by calculation without regard to physical relevance. We now show that this flux may be derived from physical considerations alone, at least for a single crystal and $\mathcal{d}$ of edge type. Consider first a single active slip system, so that

$$\boldsymbol{L}^p = \nu^\alpha(\boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha).$$

Our computation of Burgers vectors uses a right-hand screw-rule, and therefore the *natural line direction* $\boldsymbol{\ell}^\alpha$ *for edge dislocations* moving on this slip system is

$$\boldsymbol{\ell}^\alpha = \boldsymbol{m}^\alpha \times \boldsymbol{s}^\alpha, \tag{11.7}$$

because the Burgers vector associated with this line direction gives slip corresponding to material above the slip plane (i.e., in the region into which $\boldsymbol{m}^\alpha$ points) moving in the direction $\boldsymbol{s}^\alpha$ relative to material below the plane. The flux $\boldsymbol{q}$ of dislocations — as resolved on the system $\mathcal{d}$ — due to slip on α should have the following properties: (i) $\boldsymbol{q}$ should be orthogonal to the dislocation line and hence to $\boldsymbol{\ell}$, since the tangential motion of a dislocation line is irrelevant; (ii) $\boldsymbol{q}$ should lie in the slip plane and should hence be orthogonal to $\boldsymbol{m}^\alpha$; (iii) the magnitude of $\boldsymbol{q}$ should be $(\nu^\alpha \boldsymbol{s}^\alpha)\cdot\boldsymbol{b}$; (iv) for $\boldsymbol{\ell}$ the natural line direction for slip on α, the flux should be $(\boldsymbol{s}^\alpha\cdot\boldsymbol{b})\boldsymbol{s}^\alpha$. These conditions determine $\boldsymbol{q}$. Indeed, (i) and (ii) imply that $\boldsymbol{q}$ should lie on the line spanned by the unit vector $\boldsymbol{\ell}\times\boldsymbol{m}^\alpha$ and hence, by (iii), should have the form $\pm\nu^\alpha(\boldsymbol{s}^\alpha\cdot\boldsymbol{b})\,\boldsymbol{\ell}\times\boldsymbol{m}^\alpha$. By (11.7), condition (iv) requires that we take the positive sign:

$$\boldsymbol{q} = \nu^\alpha(\boldsymbol{s}^\alpha\cdot\boldsymbol{b})\,\boldsymbol{\ell}\times\boldsymbol{m}^\alpha = (\boldsymbol{\ell}\times)(\nu^\alpha\mathbb{S}^{\alpha\top})\boldsymbol{b}.$$

If we allow for the possibility of all slip systems being active, then we arrive at the following formula for the dislocation flux as measured in the microstructural configuration:

$$\boldsymbol{q}(\boldsymbol{\ell},\boldsymbol{b}) = (\boldsymbol{\ell}\times)\boldsymbol{L}^{p\top}\boldsymbol{b}. \tag{11.8}$$

11.3 Relations for $\dot{\boldsymbol{G}}$

In discussing geometrically necessary dislocations in single crystals it would seem useful to have available identities relating $\dot{\boldsymbol{G}}$ to the slips ν^α and their gradients.

By (4.6),

$$\dot{\boldsymbol{G}} = \overline{\left(\frac{1}{J^p}\boldsymbol{F}^p\right)}^{\boldsymbol{\cdot}} \operatorname{Curl}\boldsymbol{F}^p + \frac{1}{J^p}\boldsymbol{F}^p \operatorname{Curl}\dot{\boldsymbol{F}}^p, \tag{11.9}$$

while $(2.13)_2$ and (3.4) yield

$$\operatorname{Curl}\dot{\boldsymbol{F}}^p = (\operatorname{Curl}\boldsymbol{F}^p)\boldsymbol{L}^{p\top} + \operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p), \tag{11.10}$$

where $\operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p)$ is the Curl of $\boldsymbol{L}^p\boldsymbol{F}^p$ holding $\boldsymbol{F}^p$ fixed. Thus appealing to (3.4) and (3.5),

$$\dot{\boldsymbol{G}} = -(\operatorname{tr}\boldsymbol{L}^p)\boldsymbol{G} + \boldsymbol{L}^p\boldsymbol{G} + \boldsymbol{G}\boldsymbol{L}^{p\top} + \frac{1}{J^p}\boldsymbol{F}^p\operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p). \tag{11.11}$$

Because the time-derivative in (11.11) is material, a much simpler formula ensues when the geometric dislocation tensor is referred to the reference configuration. By (6.1),

$$\dot{\boldsymbol{G}}_{\mathrm{R}} = (\operatorname{Curl}\boldsymbol{F}^p)\overline{\boldsymbol{F}^{p-\top}}^{\boldsymbol{\cdot}} + (\operatorname{Curl}\dot{\boldsymbol{F}}^p)\boldsymbol{F}^{p-\top}, \tag{11.12}$$

In view of (3.4) and the identity $\overline{\boldsymbol{T}^{-1}}^{\boldsymbol{\cdot}} = -\boldsymbol{T}^{-1}\dot{\boldsymbol{T}}\boldsymbol{T}^{-1}$,

$$\overline{\boldsymbol{F}^{p-\top}}^{\boldsymbol{\cdot}} = -\boldsymbol{L}^{p\top}\boldsymbol{F}^{p-\top}, \tag{11.13}$$

and therefore, by (11.10),

$$\dot{\boldsymbol{G}}_{\mathrm{R}} = \operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p)\boldsymbol{F}^{p-\top}. \tag{11.14}$$

$\dot{\boldsymbol{G}}_{\mathrm{R}}$ therefore vanishes when $\nabla\boldsymbol{L}^p = \boldsymbol{0}$. Thus, for a single crystal, $\boldsymbol{G}_{\mathrm{R}}$ convects with the motion of the body whenever the slip-gradients vanish.

The term $\operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p)$ is, in general, complicated, but it does reduce when attention is restricted to *single crystals.* In that case $\boldsymbol{L}^p$ has the explicit form (3.16) and $\operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p)$ comes from computing

$$\operatorname{Curl}(\boldsymbol{L}^p\boldsymbol{F}^p) = \sum_{\alpha=1}^{A}\operatorname{Curl}\{\nu^\alpha\,\mathbb{S}^\alpha\boldsymbol{F}^p\} \tag{11.15}$$

holding $\boldsymbol{F}^p$ fixed, or equivalently holding $\mathbb{S}^\alpha\boldsymbol{F}^p$ fixed for each α. Thus $(2.13)_3$, (2.16), and the fact that $J^p = 1$ yield

$$\boldsymbol{F}^p\operatorname{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p) = \sum_{\alpha=1}^{A}\boldsymbol{F}^p(\nabla\nu^\alpha\times)\boldsymbol{F}^{p\top}\mathbb{S}^{\alpha\top} = \sum_{\alpha=1}^{A}\{(\boldsymbol{F}^{p-\top}\nabla\nu^\alpha)\times\}\,\mathbb{S}^{\alpha\top}.$$

Further, since $\nabla\nu^\alpha = \boldsymbol{F}^\top\operatorname{grad}\nu^\alpha$ and $\boldsymbol{F} = \boldsymbol{F}^e\boldsymbol{F}^p$,

$$\boldsymbol{F}^{p-\top}\nabla\nu^\alpha = \boldsymbol{F}^{e\top}\operatorname{grad}\nu^\alpha \stackrel{\text{def}}{=} \nabla_{\mathrm{L}}\,\nu^\alpha, \tag{11.16}$$

where $\nabla_{\mathrm{L}}\,\nu^\alpha$, which is intrinsic to the lattice, represents the gradient of ν^α transported to the lattice. The evolution equation (11.11) therefore takes the form

$$\dot{\boldsymbol{G}} = \sum_{\alpha=1}^{A}\Big[\nu^\alpha\{\mathbb{S}^\alpha\boldsymbol{G} + \boldsymbol{G}\mathbb{S}^{\alpha\top}\} - \{\boldsymbol{m}^\alpha\times\nabla_{\mathrm{L}}\,\nu^\alpha\}\otimes\boldsymbol{s}^\alpha\Big]. \tag{11.17}$$

Thus $\dot{\boldsymbol{G}}$ is *linear in the slips* ν^α *and the slip-gradients* $\nabla\nu^\alpha$, *with coefficients dependent on* $\boldsymbol{F}^p$ *and* $\operatorname{Curl}\boldsymbol{F}^p$.

11.4 Strict plane strain. Relations for $\dot{g}$

Under strict plane strain $\boldsymbol{L}^p\boldsymbol{e}=0$ and $\boldsymbol{G}=\boldsymbol{e}\otimes\boldsymbol{g}$ with $\boldsymbol{e}$ constant; the analog of (11.11) is therefore

$$\dot{\boldsymbol{g}} = (\boldsymbol{L}^p - (\mathrm{tr}\boldsymbol{L}^p)\mathbf{1})\,\boldsymbol{g} + \frac{1}{J^p}[\mathrm{Curl}_{\boldsymbol{L}^p}(\boldsymbol{L}^p\boldsymbol{F}^p)]^{\top}\mathrm{e}. \tag{11.18}$$

For a rigid-plastic material an equivalent expression in terms of the elastic rotation-angle follows upon differentiation of $(9.12)_2$ and use of (11.13):

$$\dot{\boldsymbol{g}} = -\boldsymbol{L}^{p\top}\boldsymbol{g} + \nabla_{\mathrm{L}}\dot{\vartheta}^e. \tag{11.19}$$

The specialization to single-crystals may be obtained by direct substitution of $\boldsymbol{G}=\boldsymbol{e}\otimes\boldsymbol{g}$ into (11.17):

$$\dot{\boldsymbol{g}} = \sum_{\alpha=1}^{A}\Big[(\boldsymbol{g}\cdot\boldsymbol{m}^\alpha)\nu^\alpha + (\boldsymbol{s}^\alpha\cdot\nabla_{\mathrm{L}}\,\nu^\alpha)\Big]\boldsymbol{s}^\alpha. \tag{11.20}$$

For a rigid-plastic material, $\boldsymbol{g}=\nabla_{\mathrm{L}}\,\vartheta^e$ and this expressions reduces to

$$\dot{\boldsymbol{g}} = \sum_{\alpha=1}^{A}\Big[(\boldsymbol{m}^\alpha\cdot\nabla_{\mathrm{L}}\,\vartheta^e)\nu^\alpha + (\boldsymbol{s}^\alpha\cdot\nabla_{\mathrm{L}}\,\nu^\alpha)\Big]\boldsymbol{s}^\alpha. \tag{11.21}$$

12 The invariant description of geometrically necessary dislocations

The invariant characterization of geometrically necessary dislocations requires invariance under arbitrary *compatible* changes in reference configuration, since such changes should not induce additional dislocations of that type. The chief purpose of this section is to determine what functional dependences on $\boldsymbol{F}^p$ and $\nabla\boldsymbol{F}^p$ display this invariance.

12.1 Compatible changes in reference configuration

Let $\boldsymbol{X}_0$ denote an arbitrarily prescribed material point. By a **compatible change in local reference** (at $\boldsymbol{X}_0$) we mean a smooth one-to-one mapping $\boldsymbol{Z}=\boldsymbol{Z}(\boldsymbol{X})$ of a neighborhood of $\boldsymbol{X}_0$ onto an open set in $\mathbb{R}^3$; the points $\boldsymbol{Z}$ then represent new labels for material points. We write $\hat{\nabla}$ for the gradient with respect to points $\boldsymbol{Z}$, leaving ∇ to denote the gradient with respect to $\boldsymbol{X}$. Writing

$$\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{Z})$$

for the inverse of the mapping $\boldsymbol{Z}=\boldsymbol{Z}(\boldsymbol{X})$, let

$$\boldsymbol{H} = \hat{\nabla}\boldsymbol{X} \tag{12.1}$$

and assume that $\det\boldsymbol{H}>0$.

A motion $\boldsymbol{x}=\boldsymbol{y}(\boldsymbol{X})$ has the form

$$\boldsymbol{x} = \hat{\boldsymbol{y}}(\boldsymbol{Z}) = \boldsymbol{y}(\boldsymbol{X}(\boldsymbol{Z}))$$

relative to the new reference, and its deformation gradient $\hat{\boldsymbol{F}}=\hat{\nabla}\hat{\boldsymbol{y}}$ is given by

$$\hat{\boldsymbol{F}} = \boldsymbol{F}\boldsymbol{H}. \tag{12.2}$$

The structural transformation $\boldsymbol{F}^e$ is a linear transformation from the microstructural configuration to the deformed configuration and as such is unrelated to the reference configuration. We therefore stipulate that $\boldsymbol{F}^e$ be invariant under local changes in reference. On the other hand, by (12.2) and the decomposition $\boldsymbol{F}=\boldsymbol{F}^e\boldsymbol{F}^p$, the plastic strain $\hat{\boldsymbol{F}}^p$ relative to the new reference must, for consistency, satisfy

$$\hat{\boldsymbol{F}}^p = \boldsymbol{F}^p\boldsymbol{H}, \qquad \hat{J}^p = (\det\boldsymbol{H})J^p. \tag{12.3}$$

A discussion of the geometric dislocation tensor $\boldsymbol{G}$ requires a transformation law for Curl $\boldsymbol{F}^p$. With this in mind, we apply (2.10) with the subscript 1 associated with the new reference and hence with the variable $\boldsymbol{Z}$, with the subscript 2 associated with $\boldsymbol{X}$, and with $\hat{\mathrm{Curl}}$ the curl with respect to $\boldsymbol{Z}$. The result is the transformation law

$$\hat{\mathrm{Curl}}\,\hat{\boldsymbol{F}}^p = (\det \boldsymbol{H})\boldsymbol{H}^{-1}\mathrm{Curl}\,\boldsymbol{F}^p. \tag{12.4}$$

12.2 $\boldsymbol{G}$ as an invariant descriptor

Consider a change in local reference. Then the geometric dislocation tensor

$$\boldsymbol{G} = \frac{1}{J^p}\boldsymbol{F}^p\,\mathrm{Curl}\,\boldsymbol{F}^p \tag{12.5}$$

expressed relative to the new reference is given by

$$\hat{\boldsymbol{G}} = \frac{1}{\hat{J}^p}\hat{\boldsymbol{F}}^p\,\hat{\mathrm{Curl}}\,\hat{\boldsymbol{F}}^p;$$

an immediate consequence of (12.3) and (12.4) is therefore the following:[31]

THEOREM. *The geometric dislocation tensor is invariant under compatible changes in local reference:*

$$\hat{\boldsymbol{G}} = \boldsymbol{G}. \tag{12.6}$$

This theorem begs the question: *Are there other fields — expressible in terms of $\boldsymbol{F}^p$ and $\nabla\boldsymbol{F}^p$ — that are invariant under compatible changes in local reference*? To answer this question, consider a relation

$$\Phi = \mathcal{F}(\boldsymbol{F}^p, \nabla\boldsymbol{F}^p) \tag{12.7}$$

giving the value of a field Φ at $\boldsymbol{X}_0$ when $\boldsymbol{F}^p$ and $\nabla\boldsymbol{F}^p$ are known at $\boldsymbol{X}_0$. We say that $\mathcal{F}$ is **invariant under compatible changes in local reference** if, given any such change,

$$\mathcal{F}(\hat{\boldsymbol{F}}^p, \hat{\nabla}\hat{\boldsymbol{F}}^p) = \mathcal{F}(\boldsymbol{F}^p, \nabla\boldsymbol{F}^p). \tag{12.8}$$

INVARIANCE THEOREM. *A necessary and sufficient condition that $\mathcal{F}$ be invariant under compatible changes in local reference is that it reduce to a function $\mathcal{K}$ of the geometric dislocation tensor $\boldsymbol{G}$:*

$$\mathcal{F}(\boldsymbol{F}^p, \nabla\boldsymbol{F}^p) = \mathcal{K}(\boldsymbol{G}). \tag{12.9}$$

The proof of this theorem in given in the Appendix.

REMARK. In view of the Remark at the end of Section 4, a relation $\Phi = \mathcal{F}(\boldsymbol{F}^e, \mathrm{grad}\boldsymbol{F}^e)$ (or equivalently $\Phi = \mathcal{J}(\boldsymbol{F}^{e-1}, \mathrm{grad}\boldsymbol{F}^{e-1})$) is invariant under local superposed compatible deformations of the deformed configuration if and only if it has the form $\Phi = \mathcal{K}(\boldsymbol{G})$.

13 Appendix. Technical proofs

13.1 Proof of the Local Distortion Theorem

Let $\boldsymbol{H} = \mathrm{grad}\bar{\boldsymbol{n}}\ \mathbb{P}(\bar{\boldsymbol{n}})$. Our first step will be to show that, at a given point,

$$\mathrm{skw}\,\boldsymbol{H} = 0 \iff \boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = 0. \tag{13.1}$$

Since $\bar{\boldsymbol{n}}$ is a unit vector, $(\mathrm{grad}\bar{\boldsymbol{n}})^{\mathsf{T}}\bar{\boldsymbol{n}} = 0$; thus $\boldsymbol{H} = \mathbb{P}(\bar{\boldsymbol{n}})\,\mathrm{grad}\bar{\boldsymbol{n}}\ \mathbb{P}(\bar{\boldsymbol{n}})$. By $(2.13)_4$ and (2.15), the identity (8.4) may be rewritten as $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = J^e\bar{\lambda}^2(\bar{\boldsymbol{n}}\times)\cdot(\mathrm{skw}\boldsymbol{H})$. Let $\boldsymbol{W} = \mathrm{skw}\boldsymbol{H}$. Then $\boldsymbol{W} = \boldsymbol{W}\mathbb{P}(\bar{\boldsymbol{n}})$. Moreover,

[31] A similar argument yields the invariance of $\boldsymbol{G}$ under superposed compatible elastic deformations (Davini 1986).

$\boldsymbol{W} = \boldsymbol{w}\times$ for some vector $\boldsymbol{w}$, so that $\boldsymbol{w}\times\bar{\boldsymbol{n}} = \boldsymbol{0}$ and $\boldsymbol{w} = \kappa\bar{\boldsymbol{n}}$ for some scalar κ. Assume that $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = \boldsymbol{0}$. Then $0 = (\bar{\boldsymbol{n}}\times)\cdot(\boldsymbol{w}\times) = 2\kappa$ and $\mathrm{skw}\boldsymbol{H} = \boldsymbol{0}$. Trivially, $\mathrm{skw}\boldsymbol{H} = \boldsymbol{0} \Rightarrow \boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = \boldsymbol{0}$.

Assume that Π is locally undistorted at $\boldsymbol{x}_0$. Let $\bar{M}$ be as specified in the definition containing (8.5). Choose an arbitrary curve $\boldsymbol{z}(\sigma)$ on $\bar{M}$ through $\boldsymbol{x}_0$. Then, letting $\boldsymbol{u} = d\boldsymbol{z}/d\sigma|_{\sigma=0}$,

$$\boldsymbol{0} = \left[\frac{d}{d\sigma}\{\bar{\boldsymbol{m}}(\boldsymbol{z}(\sigma)) - \bar{\boldsymbol{n}}(\boldsymbol{z}(\sigma))\}\right]_{\sigma=0} = -\{\boldsymbol{K}(\boldsymbol{x}_0) + \mathrm{grad}\,\bar{\boldsymbol{n}}(\boldsymbol{x}_0)\}\boldsymbol{u}, \tag{13.2}$$

with $\boldsymbol{K}$ the curvature tensor on $\bar{M}$. Since $\boldsymbol{z}(\sigma)$ is an arbitrary curve, $\boldsymbol{u}$ may be considered to be an arbitrary vector *tangent to* $\bar{M}$ at $\boldsymbol{x}_0$, so that

$$\boldsymbol{K}(\boldsymbol{x}_0) = -\mathrm{grad}\,\bar{\boldsymbol{n}}(\boldsymbol{x}_0)\,\mathbb{P}(\bar{\boldsymbol{n}}(\boldsymbol{x}_0)) = -\boldsymbol{H}(\boldsymbol{x}_0). \tag{13.3}$$

By a well known theorem of Gauss, $\boldsymbol{K}$ is symmetric; thus $\boldsymbol{H}$ is symmetric and (13.1) yields $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = 0$ at $\boldsymbol{x}_0$.

Conversely, assume that $\boldsymbol{n}\cdot\boldsymbol{G}\boldsymbol{n} = 0$ at $\boldsymbol{x}_0$, so that $\boldsymbol{H}$ is symmetric at $\boldsymbol{x}_0$. To complete the proof we must establish the existence of a smooth surface $\bar{M}$ through $\boldsymbol{x}_0$ such that (8.5) is satisfied. Let

$$\bar{\boldsymbol{n}}_0 = \bar{\boldsymbol{n}}(\boldsymbol{x}_0), \qquad \mathbb{P}_0 = \mathbb{P}(\bar{\boldsymbol{n}}_0), \qquad \boldsymbol{H}_0 = \boldsymbol{H}(\boldsymbol{x}_0) = \mathbb{P}_0\,(\mathrm{grad}\,\bar{\boldsymbol{n}})(\boldsymbol{x}_0)\,\mathbb{P}_0,$$

and define

$$\bar{M} = \{\boldsymbol{x} : \Phi(\boldsymbol{x}) = 0\}, \qquad \Phi(\boldsymbol{x}) = \bar{\boldsymbol{n}}_0\cdot(\boldsymbol{x}-\boldsymbol{x}_0) + \tfrac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_0)\cdot\boldsymbol{H}_0(\boldsymbol{x}-\boldsymbol{x}_0),$$

so that $\bar{M}$ is a (quadratic) surface through $\boldsymbol{x}_0$ with $\bar{\boldsymbol{m}} = \mathrm{grad}\,\Phi/|\mathrm{grad}\,\Phi|$ a unit-normal field for $\bar{M}$ consistent with $\bar{\boldsymbol{n}}(\boldsymbol{x}_0) = \bar{\boldsymbol{m}}(\boldsymbol{x}_0)$. Computing $\boldsymbol{K} = -\mathrm{grad}\bar{\boldsymbol{m}}\,\mathbb{P}(\bar{\boldsymbol{m}})$ using the symmetry of $\boldsymbol{H}_0$ yields (13.3) and hence (13.2). Thus (8.5) is satisfied. Π is therefore locally undistorted at $\boldsymbol{x}_0$.

13.2 Proof of the Invariance Theorem

Sufficiency is a corollary of the theorem containing (12.6). To establish necessity, assume that $\mathcal{F}$ is invariant under compatible changes in local reference. Without loss in generality, take $\boldsymbol{X}_0 = \boldsymbol{0}$ and restrict attention to local reference changes that map $\boldsymbol{X} = \boldsymbol{0}$ to $\boldsymbol{Z} = \boldsymbol{0}$.

Our first step is to show that $\mathcal{F}$ must reduce to a function $\mathcal{F}^*$ of $\boldsymbol{F}^p$ and $\mathrm{Curl}\,\boldsymbol{F}^p$:

$$\mathcal{F}(\boldsymbol{F}^p, \nabla\boldsymbol{F}^p) = \mathcal{F}^*(\boldsymbol{F}^p, \mathrm{Curl}\,\boldsymbol{F}^p). \tag{13.4}$$

Let $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \boldsymbol{e}_3\}$ denote an orthonormal basis. Then $\boldsymbol{F}^p$ may be written in the form

$$\boldsymbol{F}^p = \boldsymbol{e}_i\otimes\boldsymbol{f}_i, \qquad \boldsymbol{f}_i = \boldsymbol{F}^{p\top}\boldsymbol{e}_i. \tag{13.5}$$

(Recall our use of summation convention.) On the space of all smooth vector fields $\boldsymbol{g}$ there is is a one-to-one correspondence between $\mathrm{skw}\,\nabla\boldsymbol{g}$ and $\mathrm{Curl}\,\boldsymbol{g}$. Thus, since

$$\nabla\boldsymbol{F}^p = \boldsymbol{e}_i\otimes\nabla\boldsymbol{f}_i, \qquad (\mathrm{Curl}\,\boldsymbol{F}^p)^\top = \boldsymbol{e}_i\otimes\mathrm{Curl}\,\boldsymbol{f}_i$$

(cf. $(2.13)_5$), to establish (13.4), it suffices to show that

$$\mathcal{F}(\boldsymbol{F}^p,\, \boldsymbol{e}_i\otimes\nabla\boldsymbol{f}_i) = \mathcal{F}(\boldsymbol{F}^p,\, \boldsymbol{e}_i\otimes\mathrm{skw}\nabla\boldsymbol{f}_i). \tag{13.6}$$

To this end, let

$$\boldsymbol{S}_i = \mathrm{sym}\nabla\boldsymbol{f}_i(\boldsymbol{0}), \qquad \boldsymbol{g}_i = \boldsymbol{F}^{p-1}\boldsymbol{e}_i, \tag{13.7}$$

and consider the mapping defined by

$$\boldsymbol{X} = \boldsymbol{Z} - \tfrac{1}{2}(\boldsymbol{Z}\cdot\boldsymbol{S}_k\boldsymbol{Z})\,\boldsymbol{g}_k(\boldsymbol{0}). \tag{13.8}$$

Since the gradient

$$\boldsymbol{H}(\boldsymbol{Z}) = \boldsymbol{1} - \boldsymbol{g}_k(\boldsymbol{0})\otimes(\boldsymbol{S}_k\boldsymbol{Z})$$

of (13.8) satisfies $\boldsymbol{H}(\mathbf{0})=\mathbf{1}$, (13.8) defines a compatible change in local reference (in some neighborhood of $\boldsymbol{Z}=\mathbf{0}$). Next, from (12.3) it follows that under such a change in reference $\hat{\boldsymbol{f}}_i=\boldsymbol{H}^{\top}\boldsymbol{f}_i$. Thus, since $\boldsymbol{H}(\mathbf{0})=\mathbf{1}$,

$$\nabla\hat{\boldsymbol{f}}_i(\mathbf{0})=\nabla\boldsymbol{f}_i(\mathbf{0})+\nabla\big(\boldsymbol{H}^{\top}(\boldsymbol{Z})\boldsymbol{f}_i(\mathbf{0})\big)\big|_{\boldsymbol{Z}=\mathbf{0}}.$$

By $(13.5)_2$ and $(13.7)_2$, $\boldsymbol{f}_i\cdot\boldsymbol{g}_j=\delta_{ij}$; thus

$$\boldsymbol{H}^{\top}(\boldsymbol{Z})\boldsymbol{f}_i(\mathbf{0})=\boldsymbol{f}_i(\mathbf{0})-\boldsymbol{S}_i\boldsymbol{Z},\qquad \nabla\hat{\boldsymbol{f}}_i(\mathbf{0})=\nabla\boldsymbol{f}_i(\mathbf{0})-\boldsymbol{S}_i=\mathrm{skw}\nabla\boldsymbol{f}_i(\mathbf{0}).$$

Thus, since $\hat{\boldsymbol{F}}^p(\mathbf{0})=\boldsymbol{F}^p(\mathbf{0})$, (12.8) implies (13.6). Therefore (13.4) is satisfied.

To establish (12.9), note that, by (12.8) and (13.4), $\mathcal{F}^*$ must satisfy

$$\mathcal{F}^*(\boldsymbol{F}^p,\mathrm{Curl}\,\boldsymbol{F}^p)=\mathcal{F}^*(\hat{\boldsymbol{F}}^p,\hat{\mathrm{Curl}}\,\hat{\boldsymbol{F}}^p). \tag{13.9}$$

Consider the *homogeneous* change in reference with gradient $\boldsymbol{H}\equiv\boldsymbol{F}^{p-1}(\mathbf{0})$. In this case (12.2), (12.4), and (12.5) yield $\hat{\boldsymbol{F}}^p(\mathbf{0})=\mathbf{1}$ and $\hat{\mathrm{Curl}}\,\hat{\boldsymbol{F}}^p(\mathbf{0})=\boldsymbol{G}(\mathbf{0})$, so that (13.9) reduces to $\mathcal{F}^*(\mathbf{1},\boldsymbol{G})$. Thus (13.4) reduces to (12.9).

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