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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 $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$. The incompatibility of $\mathbf{F}^e$ and that of $\mathbf{F}^p$ are characterized by a single tensor $\mathbf{G}$ giving the Burgers vector, measured and reckoned per unit area in the microstructural (intermediate) configuration. We show that $\mathbf{G}$ may be expressed in terms of $\mathbf{F}^p$ and the referential curl of $\mathbf{F}^p$, or *equivalently* in terms of $\mathbf{F}^{e-1}$ and the spatial curl of $\mathbf{F}^{e-1}$. We derive explicit relations for $\mathbf{G}$ 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 $\mathbf{G}$ and the distortion of microstructural planes. We show that kinematics alone yields a balance law for the transport of geometrically necessary dislocations. © 2001 Published by Elsevier Science Ltd.

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1. Introduction

Modern treatments of finite plasticity are based on the Kröner (1960) — Lee (1969) decomposition $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$ of the deformation gradient $\mathbf{F} = \nabla\mathbf{y}$ into structural (elastic) and plastic components, where $\mathbf{x} = \mathbf{y}(\mathbf{X}, t)$ represents the deformation that carries material points $\mathbf{X}$ in the reference configuration into their positions $\mathbf{x}$ at time t in the deformed configuration. For a single crystal, $\mathbf{F}^p(\mathbf{X})$ represents the "local deformation" of *referential* line segments to line segments $d\mathbf{l} = \mathbf{F}^p(\mathbf{X})\,d\mathbf{X}$ in the *microstructural* (*or lattice*) *configuration*, a deformation resulting solely from the formation of defects

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such as dislocations; $\mathbf{F}^e(\mathbf{X})$ represents the "local deformation" of the segments $\mathrm{d}\mathbf{l}$ into segments $\mathrm{d}\mathbf{x} = \mathbf{F}^e(\mathbf{X})\,\mathrm{d}\mathbf{l}$ due to stretching and rotation of the *lattice*.

An important feature of the Kröner–Lee decomposition is that, while $\mathbf{F}$ is *compatible* (the gradient of a vector field), $\mathbf{F}^e$ and $\mathbf{F}^p$ 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 possible to characterize such dislocations through a tensor field $\mathbf{G}$ 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.

With the exception of Subsection 2.1,

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

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

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

denote the divergence, gradient, and curl with respect to the point $\mathbf{x} = \mathbf{y}(\mathbf{X}, t)$ in the *deformed configuration*; $\dot{\varphi}$ denotes the *material time derivative* (holding $\mathbf{X}$ fixed).

1.1. 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 $\mathbf{e}_k(\mathbf{x})$. These fields are viewed as the generators, on a microscopic scale, of a Bravais lattice deformed via a tensor field $\mathbf{A}(\mathbf{x})$ through a transformation $\mathbf{e}_k(\mathbf{x}) = \mathbf{A}(\mathbf{x})\mathbf{c}_k$ of a basis $\mathbf{c}_k$ of a fixed reference lattice $\mathscr{L}$. 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 the Kröner–Lee decomposition upon identifying the elastic deformation tensor $\mathbf{F}^e$ with $\mathbf{A}$. 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

$$\mathbf{G}^e_{\mathrm{Ko}} = J^e \mathbf{F}^{e-1}\,\mathrm{curl}\,\mathbf{F}^{e-1} \tag{1.1}$$

with $J^e = \det \mathbf{F}^e$. 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

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

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

$$\mathrm{curl}\ \mathbf{F}^e\mathbf{F}^{e-\mathrm{T}},\ \mathrm{curl}\ \mathbf{F}^e,\ \mathbf{F}^{e-1}\ \mathrm{curl}\ \mathbf{F}^{e-1},\ \text{and}\ \mathbf{R}^{e\mathrm{T}}\ \mathrm{curl}\ \mathbf{F}^{e-1} \tag{1.2}$$

as measures of GNDs in finite deformations.

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

$$\mathbf{G}^e_{\mathrm{Kr}} = \mathrm{curl}\,\mathbf{F}^{e-1}\mathbf{F}^{e\mathrm{T}} \quad \text{and} \quad \mathbf{G}^p_{\mathrm{Kr}} = \mathrm{Curl}\,\mathbf{F}^p. \tag{1.3}$$

Kröner then goes on to develop a complete theory within the context of infinitesimal displacements, where $\mathbf{G}^e_{\mathrm{Kr}} = \mathbf{G}^p_{\mathrm{Kr}}$. 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:

(i) $\mathbf{G}$ should measure the local Burgers vector in the microstructural configuration, per unit area in that configuration;
(ii) $\mathbf{G}$ should, at any point, be expressible in terms of the *field* $\mathbf{F}^p$ *in a neighborhood of the point*, since, by fiat, $\mathbf{F}^p$ characterizes the defect structure near the point in question;
(iii) $\mathbf{G}$ 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.

Note that conditions (ii) and (iii) trivially render $\mathbf{G}$ frame-indifferent; of (1.2), only $(1.2)_{3,4}$ are frame-indifferent. It is clear from the work of Teodosiu (1970, 1982) and Davini (1986) that the measure $\mathbf{G}^e_{\mathrm{Ko}}$ satisfies (i) and (iii), but (ii) would seem problematic. On the other hand, $\mathbf{G}^p_{\mathrm{Kr}}$ trivially satisfies (ii), but violates (i). The remaining measures listed in (1.2) violate (i) and (iii). Teodosiu (1970, 1982) noted that $\mathbf{G}^{e\mathrm{T}}_{\mathrm{Ko}}\mathbf{n}$ represents the Burgers vector — measured in the reference lattice — for an infinitesimal circuit in $\mathscr{L}$ enclosing a surface element with unit normal $\mathbf{n}$. Davini (1986) showed that $\mathbf{G}^e_{\mathrm{Ko}}$ is invariant under superposed compatible elastic deformations (cf. Davini and Parry, 1989; Cermelli and Sellers, 2000). Finally, Noll (1967) was led to $\mathbf{G}^e_{\mathrm{Ko}}$ in his theory of materially uniform simple bodies with inhomogeneities, $\mathbf{G}^p_{\mathrm{Kr}}$ was used by Naghdi and Srinivasa (1993), and $\mathbf{G}^e_{\mathrm{Kr}}$ was used by Dłużewski (1996).

1.2. The geometric dislocation tensor $\mathbf{G}$

Our main result is the existence of a tensorial measure of GNDs, the *geometric dislocation tensor* $\mathbf{G}$, consistent with requirements (i)–(iii) stated above. In physical terms,

> $\mathbf{G}^{\mathrm{T}}\mathbf{n}$ *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* $\mathbf{n}$.

We refer to $\mathbf{G}^{\mathrm{T}}\mathbf{n}$ as *the Burgers vector for* Π. What is most important, $\mathbf{G}$ may be expressed in a form

$$\mathbf{G} = \frac{1}{J^p}\mathbf{F}^p \,\mathrm{Curl}\,\mathbf{F}^p, \tag{1.4}$$

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

$$\mathbf{G} = J^e\mathbf{F}^{e-1}\,\mathrm{curl}\,\mathbf{F}^{e-1}, \tag{1.5}$$

that depends only on the field $\mathbf{F}^e$. Because we do *not* require that $\det\mathbf{F}^p = 1$, our discussion allows for the formation of voids and the interaction of voids with other defects.

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

(i) For situations in which lattice strains are small, GNDs would seem amenable to experimental study through measurement of lattice rotations (cf. Sun et al., 1998, 2000); the relation for $\mathbf{G}$ in terms of $\mathbf{F}^e$ (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 $\mathbf{G}$ in terms of $\mathbf{F}^p$, which characterizes defects, leaving $\mathbf{F}^e$ to describe the stretching and rotation of the lattice. The importance of the relation for $\mathbf{G}$ in terms of $\mathbf{F}^p$ is underlined by a relation we derive giving $\dot{\mathbf{G}}$ for a single crystal as a function of $\mathbf{F}^p$, $\mathrm{Curl}\,\mathbf{F}^p$, the slips, and the slip gradients.

Given a fixed unit vector $\mathbf{n}$, consider the microstructural plane Π normal to $\mathbf{n}$. We show that $\mathbf{n}\cdot\mathbf{G}(\mathbf{x})\mathbf{n}$ — the normal component of the Burgers vector for Π — is related to the *distortion* of Π. Precisely, we show that $\mathbf{n}\cdot\mathbf{G}\mathbf{n} = 0$ everywhere if and only if Π is *undistorted*; that is, if and only if Π convects to a family of smooth surfaces in the deformed configuration. The field $\mathbf{n}\cdot\mathbf{G}\mathbf{n}$ might therefore be useful as a constitutive quantity related to hardening due to the formation of GNDs. This field, which we term the "distortion modulus", accounts for the normal component of the Burgers vector of those dislocations impinging transversally on 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).

When elastic strains are negligible, so that $\mathbf{F}^e$ is a rotation $\mathbf{R}^e$, GNDs are amenable to experimental study through the measurement of lattice rotations as described by

$\mathbf{R}^e$. Material scientists typically describe rotations by means of Euler angles via a decomposition of the form

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

in which the $\mathbf{c}_i$ are constant unit vectors and $\mathbf{Q}(\vartheta_i(\mathbf{x}), \mathbf{c}_i)$ represents a counterclockwise rotation about $\mathbf{c}_i$ through an angle $\vartheta_i(\mathbf{x})$. As one of our main results we show that the geometric dislocation tensor $\bar{\mathbf{G}} = \mathbf{R}^e\mathbf{G}\mathbf{R}^{e\mathrm{T}}$ referred to the deformed configuration has the simple form

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

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

1.3. Strict plane strain and strict anti-plane shear

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

For strict plane strain $\mathbf{G}$ is a "pure edge tensor"

$$\mathbf{G} = \mathbf{e} \otimes \mathbf{g}, \quad \mathbf{g} \perp \mathbf{e}$$

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

$$\mathbf{g} = \mathbf{R}^{e\mathrm{T}} \operatorname{grad}\vartheta^e.$$

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

For strict anti-plane shear with $\mathbf{e}$ the unit vector that defines the shear axis, $\mathbf{F}^p = \mathbf{1} + \mathbf{e} \otimes \gamma^p$, with γ^p orthogonal to $\mathbf{e}$, and the geometric dislocation tensor is a "pure screw tensor"

$$\mathbf{G} = \mathbf{e} \otimes \mathbf{h}, \quad \mathbf{h} = \operatorname{curl}\gamma^p, \quad \mathbf{h} \| \mathbf{e}.$$

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

1.4. Dynamics

Kinematics alone yields a balance law for the transport of GNDs. Consider a prescribed microstructural plane Π with unit normal $\mathbf{l}$ and a prescribed unit vector $\mathbf{b}$, which need bear no relation to $\mathbf{l}$. Then $\rho(\ell, \mathbf{b}) = \mathbf{l} \cdot \mathbf{G}\mathbf{b}$ is the component in the direction $\mathbf{b}$ of the Burgers vector, per unit area, on Π. We show that any such (signed) *density*[1] $\rho = \rho(\mathbf{l}, \mathbf{b})$ evolves in accord with the *balance law*

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

with dislocation flux $\mathbf{q}_{\mathrm{R}}$ and dislocation supply σ_{R} defined by

$$\mathbf{q}_{\mathrm{R}} = \mathbf{F}^{p-1}(\mathbf{l} \times (\mathbf{L}^{p\mathrm{T}}\mathbf{b})),\ \sigma_{\mathrm{R}} = \mathbf{l} \cdot \mathbf{L}^{p}\mathbf{G}\mathbf{b} + \mathbf{b} \cdot \mathbf{L}^{p}\mathbf{G}\mathbf{l},$$

where $\mathbf{L}^p = \dot{\mathbf{F}}^p\mathbf{F}^{p-1}$. This balance is one of our main results; one of its more interesting consequences is that plastic flow, as characterized by non-vanishing values of $\mathbf{L}^p$, is always associated with a flux of dislocations, whether or not $\mathbf{G}$ vanishes. Here we emphasize that $\mathbf{G}$ — and hence the density ρ — accounts only for GNDs, as it measures the *net* dislocation density associated with macroscopic incompatibility.

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

2. Preliminaries

2.1. Mappings of surfaces

Let $\mathbf{h}$ be a smooth one-to-one mapping of a region D_1 of $\mathbb{R}^3$ onto another such region D_2, with $\mathbf{H} = \nabla\mathbf{h}$, $\det\mathbf{H} > 0$. Further, let $S_i \subset D_i$ $(i = 1, 2)$ be smooth surfaces with $S_2 = \mathbf{h}(S_1)$, and with S_i oriented by a smooth unit-normal field $\mathbf{n}_i$. Then, modulo a change in the sign of $\mathbf{n}_2$,

$$\mathbf{n}_2 = \frac{\mathbf{H}^{-\mathrm{T}}\mathbf{n}_1}{|\mathbf{H}^{-\mathrm{T}}\mathbf{n}_1|}, \tag{2.1}$$

where $\mathbf{H}^{-\mathrm{T}} = (\mathbf{H}^{\mathrm{T}})^{-1}$. The *surface jacobian* of $\mathbf{h}$ as a mapping of S_1 onto S_2 is given by $\jmath = (\det\mathbf{H})|\mathbf{H}^{-\mathrm{T}}\mathbf{n}_1|$, so that, for f a scalar field and $\mathbf{T}$ a tensor field,

$$\int_{S_2} f\,\mathrm{d}A_2 = \int_{S_1} f\jmath\,\mathrm{d}A_1,\quad \int_{S_2} \mathbf{T}\mathbf{n}_2\,\mathrm{d}A_2 = \int_{S_1} (\det\mathbf{H})\mathbf{T}\mathbf{H}^{-\mathrm{T}}\mathbf{n}_1\,\mathrm{d}A_1 \tag{2.2}$$

with $\mathrm{d}A_i$ the area measure on S_i. (More precisely, if the domain of $\mathbf{T}$ is D_1, then the integral over D_2 should involve the composition $\mathbf{T} \circ \mathbf{h}$; similarly for f.) We refer to the vector measures $\mathbf{n}_i\,\mathrm{d}A_i$ $(i = 1, 2)$ as *surface elements* with unit normal $\mathbf{n}_i$ and area $\mathrm{d}A_i$. Since the fields f and $\mathbf{T}$ are arbitrary, we view (2.2), formally, as asserting that the surface element $\mathbf{n}_1\,\mathrm{d}A_1$ on S_1 is mapped by $\mathbf{h}$ into the surface element

$$\mathbf{n}_2\,\mathrm{d}A_2 = (\det\mathbf{H})\mathbf{H}^{-\mathrm{T}}\mathbf{n}_1\,\mathrm{d}A_1 \tag{2.3}$$

[1] An alternative approach to the modeling of dislocations has been suggested by Nye (1953). Noting that the Burgers vector 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 $\mathbf{G}$, but $\mathbf{G}$ does not uniquely characterize the elementary densities. For instance, in the "fcc-deconstruction" (Sun et al., 1998, 2000) there are 18 elementary densities (cf. footnote 2), but only 9 independent components of $\mathbf{G}$, a difficulty overcome by a minimization technique that furnishes a lower bound for the total density.

on S_2 (with area element $\mathrm{d}A_1$ mapped into $\mathrm{d}A_2 = \jmath\,\mathrm{d}A_1$ and $\mathbf{n}_1$ mapped into $\mathbf{n}_2$ via (2.1)).

2.2. The curl operator. Stokes theorem. The skew tensor $\mathbf{w}\times$

This subsection concerns tensor analysis in $\mathbb{R}^3$ with ∇ and curl the underlying gradient and curl operators.

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

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

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

$$\int_\Gamma \mathbf{f}\cdot \mathrm{d}\mathbf{x} = \int_S (\operatorname{curl}\mathbf{f})\cdot\mathbf{n}\,\mathrm{d}A. \tag{2.4}$$

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

$$\int_\Gamma \mathbf{T}\,\mathrm{d}\mathbf{x} = \int_S (\operatorname{curl}\mathbf{T})^{\mathrm{T}}\mathbf{n}\,\mathrm{d}A. \tag{2.5}$$

The verification of (2.5) is immediate: simply apply (2.4) with $\mathbf{f}=\mathbf{T}^{\mathrm{T}}\mathbf{c}$ and $\mathbf{c}$ constant.

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

$$(\operatorname{curl}\mathbf{T})_{ij} = \varepsilon_{irs}\frac{\partial T_{js}}{\partial x_r}$$

with ε_{irs} the alternating symbol. (A cautionary note: for some authors the curl of $\mathbf{T}$ is the transpose of our $\operatorname{curl}\mathbf{T}$.)

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

$$\mathbb{P}(\mathbf{e}) = \mathbf{1} - \mathbf{e}\otimes\mathbf{e} \tag{2.6}$$

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

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

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

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

$$(\mathbf{w}\times)(\mathbf{u}\times) = \mathbf{u}\otimes\mathbf{w} - (\mathbf{u}\cdot\mathbf{w})\mathbf{1}, \tag{2.7}$$

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

$$\mathbf{W} = \mathbf{w}\times.$$

Let v be a scalar field, let $\mathbf{f}$ and $\mathbf{u}$ be vector fields, let $\mathbf{S}$ and $\mathbf{T}$ be tensor fields with $\mathbf{T}$ constant, and let $\mathbf{a}$ be a constant vector. The following *identities* will be useful:

$$\begin{aligned}
&\operatorname{curl}\nabla\mathbf{f} = \mathbf{0},\\
&\operatorname{curl}(\mathbf{TS}) = (\operatorname{curl}\mathbf{S})\mathbf{T}^{\mathrm{T}},\\
&\operatorname{curl}(v\mathbf{T}) = (\nabla v\times)\mathbf{T}^{\mathrm{T}},\\
&\mathbf{a}\cdot\operatorname{curl}\mathbf{f} = (\mathbf{a}\times)\cdot\nabla\mathbf{f},\\
&\operatorname{curl}(\mathbf{u}\otimes\mathbf{f}) = (\operatorname{curl}\mathbf{f})\otimes\mathbf{u} - (\mathbf{f}\times)(\nabla\mathbf{u})^{\mathrm{T}},\\
&\operatorname{curl}(\mathbf{f}\times) = (\operatorname{div}\mathbf{f})\mathbf{1} - \nabla\mathbf{f}.
\end{aligned} \tag{2.8}$$

Moreover, if rather than being a constant, $\mathbf{T}(v)$ is a function of v, then

$$\operatorname{curl}(\mathbf{TS}) = (\operatorname{curl}\mathbf{S})\mathbf{T}^{\mathrm{T}} + (\nabla v\times)\left(\frac{\mathrm{d}\mathbf{T}}{\mathrm{d}v}\mathbf{S}\right)^{\mathrm{T}}. \tag{2.9}$$

To establish these identities note first that, for $\mathbf{c}$ a constant vector,

$$\begin{aligned}
&(\operatorname{curl}\nabla\mathbf{f})\mathbf{c} = \operatorname{curl}\{(\nabla\mathbf{f})^{\mathrm{T}}\mathbf{c}\} = \operatorname{curl}\nabla(\mathbf{f}\cdot\mathbf{c}) = \mathbf{0},\\
&\{\operatorname{curl}(\mathbf{TS})\}\mathbf{c} = \operatorname{curl}\{\mathbf{S}^{\mathrm{T}}(\mathbf{T}^{\mathrm{T}})\mathbf{c})\} = (\operatorname{curl}\mathbf{S})\mathbf{T}^{\mathrm{T}}\mathbf{c},\\
&\{\operatorname{curl}(v\mathbf{T})\}\mathbf{c} = \operatorname{curl}(v\,\mathbf{T}^{\mathrm{T}}\mathbf{c}) = (\nabla v\times)\mathbf{T}^{\mathrm{T}}\mathbf{c},
\end{aligned}$$

which verifies $(2.8)_{1-3}$. Identity $(2.8)_4$ follows from the definitions of curl and $\mathbf{a}\times$. Identity $(2.8)_5$ follows from the computation

$$\begin{aligned}
\{\operatorname{curl}(\mathbf{u}\otimes\mathbf{f})\}\mathbf{c} &= \operatorname{curl}\{(\mathbf{c}\cdot\mathbf{u})\mathbf{f}\} = (\mathbf{c}\cdot\mathbf{u})(\operatorname{curl}\mathbf{f}) - \mathbf{f}\times\nabla(\mathbf{c}\cdot\mathbf{u})\\
&= \{(\operatorname{curl}\mathbf{f})\otimes\mathbf{u} - (\mathbf{f}\times)(\nabla\mathbf{u})^{\mathrm{T}}\}\mathbf{c},
\end{aligned}$$

while $(2.8)_6$ is a consequence of the relation $\{\operatorname{curl}(\mathbf{f}\times)\}\mathbf{c} = \operatorname{curl}(\mathbf{c}\times\mathbf{f})$ and standard vector identities.

Assume next that $\mathbf{T} = \mathbf{T}(v)$. The curl of $\mathbf{TS}$ is the curl holding $\mathbf{T}$ fixed plus the curl holding $\mathbf{S}$ fixed. Denoting the latter by $\operatorname{curl}_{\mathbf{T}}$, we may use $(2.8)_2$ to conclude that

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

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

$$\{\operatorname{curl}_{\mathbf{T}}(\mathbf{TS})\}\mathbf{c} = \operatorname{curl}_{\mathbf{T}}\{(\mathbf{TS})^{\mathrm{T}}\mathbf{c}\} = (\nabla v\times)\left(\frac{\mathrm{d}\mathbf{T}}{\mathrm{d}v}\mathbf{S}\right)^{\mathrm{T}}\mathbf{c},$$

so that $\operatorname{curl}_{\mathbf{T}}(\mathbf{TS}) = (\nabla v\times)((\mathrm{d}\mathbf{T}/\mathrm{d}v)\mathbf{S})^{\mathrm{T}}$, which yields (2.9).

The tensor $\mathbf{e}\times$ satisfies $\mathbf{e}\times = \mathbb{P}(\mathbf{e})(\mathbf{e}\times)\mathbb{P}(\mathbf{e})$. Thus, since $\mathbf{e}\times$ is skew and $\mathbb{P}(\mathbf{e})$ symmetric, we have the identity

$$(\mathbf{e}\times)\cdot\mathbf{S} = (\mathbf{e}\times)\cdot\{\,\mathbb{P}(\mathbf{e})\mathbf{S}\,\mathbb{P}(\mathbf{e})\} = (\mathbf{e}\times)\cdot\operatorname{skw}\{\mathbb{P}(\mathbf{e})\mathbf{S}\mathbb{P}(\mathbf{e})\} \tag{2.10}$$

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

$$\operatorname{sym}\mathbf{S} = \tfrac{1}{2}(\mathbf{S}+\mathbf{S}^{\mathrm{T}}),\quad \operatorname{skw}\mathbf{S} = \tfrac{1}{2}(\mathbf{S}-\mathbf{S}^{\mathrm{T}}).$$

Finally, since $(\det \mathbf{T})\varepsilon_{ijk} = \varepsilon_{pqr}T_{ip}T_{jq}T_{kr}$, it follows that, for $\mathbf{T}$ invertible,

$$\mathbf{T}(\mathbf{b}\times)\mathbf{T}^{\mathrm{T}} = (\det \mathbf{T})(\mathbf{T}^{-\mathrm{T}}\mathbf{b}) \times . \tag{2.11}$$

3. Basic kinematics

3.1. Macroscopic kinematics. Plastic strain. Structural deformation tensor

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

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

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

with *deformation gradient*

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

consistent with $J = \det \mathbf{F} > 0$.

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

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

where $\mathbf{F}^p$, the *plastic strain*, represents the distortion of material elements due to the formation of defects in the microscopic structure, while $\mathbf{F}^e$, the *structural deformation tensor*, represents *stretching and rotation* of this structure. Unlike $\mathbf{F}$, the tensors $\mathbf{F}^p$ and $\mathbf{F}^e$ do not generally correspond to deformations (i.e., are not gradients of vector fields), but because $\mathbf{F}^p$ and $\mathbf{F}^e$ 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 $\mathbf{F}^p$ locally to reference increments $\mathrm{d}\mathbf{X}$ or, equivalently, by applying $\mathbf{F}^{e-1}$ locally to increments $\mathrm{d}\mathbf{x}$. By (3.2),

$$J = J^eJ^p, \quad J^e = \det \mathbf{F}^e, \quad J^p = \det \mathbf{F}^p \tag{3.3}$$

and we assume, without loss in generality, that $J^e > 0$ and $J^p > 0$. For specificity, we consider the microstructural fields $\mathbf{F}^e$, $\mathbf{F}^p$, J^e, and J^p as functions of $\mathbf{X}$ on B_{R}.

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

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

represents the *plastic strain rate*, measured in the microstructural configuration. A standard identity then yields the analogous relation $\dot{J}^p = J^p \operatorname{tr} \mathbf{L}^p$. Particular microscopic structures are often characterized by restrictions on the form of the tensor $\mathbf{L}^p$.

The polar decompositions

$$\mathbf{F}^p = \mathbf{R}^p\mathbf{U}^p = \mathbf{V}^p\mathbf{R}^p,$$
$$\mathbf{F}^e = \mathbf{R}^e\mathbf{U}^e = \mathbf{V}^e\mathbf{R}^e \tag{3.5}$$

define the plastic and elastic rotations $\mathbf{R}^p$ and $\mathbf{R}^e$, the plastic and elastic right-stretch tensors $\mathbf{U}^p$ and $\mathbf{U}^e$, and the plastic and elastic left-stretch tensors $\mathbf{V}^p$ and $\mathbf{V}^e$. 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

$$\mathbf{U}^e = \mathbf{V}^e = \mathbf{1} \quad (\text{so that } \mathbf{F}^e = \mathbf{R}^e,\ J^e = 1). \tag{3.6}$$

3.2. 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*

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

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

$$\bar{\mathbf{n}} = \frac{\mathbf{F}^{-\mathrm{T}}\mathbf{n}_{\mathrm{R}}}{|\mathbf{F}^{-\mathrm{T}}\mathbf{n}_{\mathrm{R}}|} \tag{3.7}$$

(cf. (2.1)); the surface element $\mathbf{n}_{\mathrm{R}}\,\mathrm{d}A_{\mathrm{R}}$ on S_{R} convects to the surface element $\bar{\mathbf{n}}\,\mathrm{d}\bar{A}$ on $\bar{S}$ defined by

$$\bar{\mathbf{n}}\,\mathrm{d}\bar{A} = J\mathbf{F}^{-\mathrm{T}}\mathbf{n}_{\mathrm{R}}\,\mathrm{d}A_{\mathrm{R}} \tag{3.8}$$

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

(a) $\{\ldots\}_{\mathrm{R}}$ denotes its representation in the reference configuration;
(b) $\{\ldots\}$ (no embellishments) denotes its representation in the microstructural configuration;
(c) $\overline{\{\ldots\}}$ 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 $\bar{B}$ is the deformed body), but in each case the quantities will be consistent with our use of the term "convect" in the sense that $\{\ldots\}$ *convects from* $\{\ldots\}_{\mathrm{R}}$ and *convects to* $\overline{\{\ldots\}}$, and so forth.

The ambient space of the microstructural configuration consists of a collection of copies of $\mathbb{R}^3$, one copy $\mathscr{L}(\mathbf{X})$ for each material point $\mathbf{X}$. $\mathscr{L}(\mathbf{X})$ should be viewed as the ambient space into which an infinitesimal neighborhood of $\mathbf{X}$ is carried by the linear transformation $\mathbf{F}^p(\mathbf{X})$ — or to which an infinitesimal neighborhood of $\mathbf{x}=\mathbf{y}(\mathbf{X})$ is carried backwards by $\mathbf{F}^{e-1}(\mathbf{x})$. (Throughout, we use abbreviations such as $\mathbf{F}^{e-1}=(\mathbf{F}^e)^{-1}$

and $\mathbf{F}^{p-\mathrm{T}} = (\mathbf{F}^p)^{-\mathrm{T}}$.) The operation of integration is physically meaningless on $\mathscr{L}(\mathbf{X})$, as integration is *not local*, but the notion of a surface element $\mathbf{n}\,dA$ (with unit normal $\mathbf{n}$ and area dA) does have meaning, as $\mathbf{n}\,dA$ is *local*. Thus, bearing in mind the paragraph containing (2.3), we *formally* stipulate that a unit normal $\mathbf{n}_\mathrm{R}$ and surface element $\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R}$ at $\mathbf{X}$ convect to the unit normal and surface element

$$\mathbf{n} = \frac{\mathbf{F}^{p-\mathrm{T}}\mathbf{n}_\mathrm{R}}{|\mathbf{F}^{p-\mathrm{T}}\mathbf{n}_\mathrm{R}|} \quad \text{and} \quad \mathbf{n}\,\mathrm{d}A = J^p\mathbf{F}^{p-\mathrm{T}}\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R} \tag{3.9}$$

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

$$\bar{\mathbf{n}} = \frac{\mathbf{F}^{e-\mathrm{T}}\mathbf{n}}{|\mathbf{F}^{e-\mathrm{T}}\mathbf{n}|} \quad \text{and} \quad \bar{\mathbf{n}}\,\mathrm{d}\bar{A} = J^e\mathbf{F}^{e-\mathrm{T}}\mathbf{n}\,dA \tag{3.10}$$

at $\mathbf{x}$ in the deformed configuration. Since $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$, $(3.9)_2$ and $(3.10)_2$ are consistent with (3.8). It suffices to consider relations $(3.9)_2$ and $(3.10)_2$ 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.

3.3. *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 $\alpha = 1, 2, \ldots, A$, with each system α defined by a *slip direction* $\mathbf{s}^\alpha$ and a *slip-plane normal* $\mathbf{m}^\alpha$, where

$$\mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0, \quad |\mathbf{s}^\alpha|, |\mathbf{m}^\alpha| = 1, \quad \mathbf{s}^\alpha, \mathbf{m}^\alpha = \text{constant}. \tag{3.11}$$

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

$$\mathbb{S}^\alpha = \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \tag{3.12}$$

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 $\mathbf{F}^p$ be governed by *slips* (microshear-rates) v^α on the individual slip systems via the flow rule

$$\mathbf{L}^p = \sum_{\alpha=1}^{A} v^\alpha(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) = \sum_{\alpha=1}^{A} v^\alpha\,\mathbb{S}^\alpha. \tag{3.13}$$

By $(3.11)_1$ and (3.13), $\mathrm{tr}\,\mathbf{L}^p = 0$ and a consequence of the differential equation $\dot{J}^p = J^p\,\mathrm{tr}\,\mathbf{L}^p$ is that $J^p = 1$ for all time if $J^p = 1$ initially.

3.4. *Isochoric $\mathbf{F}^p$. Decomposition for $\mathbf{F}^p$ non-isochoric*

To characterize internal damage due solely to the formation of voids one might restrict the plastic strain to a *dilatation*,

$$\mathbf{F}^p = \lambda^{-1}\mathbf{1}, \quad J^p = \lambda^{-3} \tag{3.14}$$

with λ the stretch from the microstructural configuration to the reference; (3.4) then yields the flow rule

$$\mathbf{L}^p = \upsilon \mathbf{1}, \quad \upsilon = -\dot{\overline{\ln \lambda}}. \tag{3.15}$$

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

$$\mathbf{F}^p = \lambda^{-1}\mathbf{F}_0^p, \quad J^p = \lambda^{-3}, \tag{3.16}$$

of a dilatation $\lambda^{-1}\mathbf{1}$ and a plastic strain $\mathbf{F}_0^p$ that is *isochoric* in the sense that $\det \mathbf{F}_0^p = 1$. Then, by (3.4), the plastic flow, as represented by $\mathbf{L}^p$, admits the *additive* decomposition

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

into dilatational and isochoric flows as represented by $\upsilon\mathbf{1}$, $\upsilon = -\dot{\overline{\ln \lambda}}$, and $\mathbf{L}_0^p = \dot{\mathbf{F}}_0^p \mathbf{F}_0^{p-1}$ with $\operatorname{tr} \mathbf{L}_0^p = 0$. This decomposition with $\mathbf{L}_0^p$ in the form (3.13) would represent the *interaction of slip with void-formation in single crystals.*

3.5. Plane strain. Strict plane strain

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

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

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

$$\mathbf{F} = \mathbb{P}(\mathbf{e})\mathbf{F}\mathbb{P}(\mathbf{e}) + \mathbf{e} \otimes \mathbf{e}, \quad \mathbf{L} = \mathbb{P}(\mathbf{e})\mathbf{L}\mathbb{P}(\mathbf{e}), \quad \mathbf{e} \equiv \mathbf{e}_3, \tag{3.17}$$

so that their component matrices have the respective forms

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

Tensor fields that are independent of X_3 and of the form $(3.17)_1$ are termed *planar*. Note that this definition excludes $\mathbf{L}$, which annihilates vectors parallel to $\mathbf{e}$.

The constraint of plane strain does not generally render $\mathbf{F}^p$ and $\mathbf{F}^e$ planar tensors. Indeed, for a rigid-plastic material, the polar decomposition (3.5) yields $\mathbf{F} = (\mathbf{R}^e\mathbf{R}^p)\mathbf{U}^p$ with $\mathbf{U}^p$ the square root of $\mathbf{F}^{\mathrm{T}}\mathbf{F}$; hence $\mathbf{U}^p$ and $\mathbf{R}^e\mathbf{R}^p$ must be planar, but individually $\mathbf{R}^e$ and $\mathbf{R}^p$ need not be planar.

A direct consequence of (3.4) is that, if $\mathbf{F}^p$ is planar at some time, then $\mathbf{F}^p$ and (hence) $\mathbf{F}^e$ are planar if and only if $\mathbf{L}^p\mathbf{e} = \mathbf{L}^{p\mathrm{T}}\mathbf{e} = \mathbf{0}$ (so that $\mathbf{L}^p$ has the form $(3.17)_2$). We use the term *strict plane strain* to describe plane strain with $\mathbf{F}^p$ and $\mathbf{F}^e$ *planar tensor fields*. Under strict plane strain, $\mathbf{F}^p\mathbf{e} = \mathbf{e}$ and $\mathbf{F}^{p\mathrm{T}}\mathbf{e} = \mathbf{e}$, and similarly for $\mathbf{F}^e$ (and $\mathbf{F}$); hence *referential planes perpendicular to* $\mathbf{e}$ *convect to planes perpendicular to* $\mathbf{e}$ *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*; that is, slip systems α that satisfy

$$\mathbf{s}^\alpha \cdot \mathbf{e} = 0, \quad \mathbf{m}^\alpha \cdot \mathbf{e} = 0, \quad \mathbf{s}^\alpha \times \mathbf{m}^\alpha = \mathbf{e} \tag{3.18}$$

with slips ν^α independent of X_3. 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; Prantil et al., 1993. Cf. also Kalinindi and Anand (1993) who discuss plane strain allowing for a full three-dimensional collection of slip systems.)

4. Burgers vector. The geometric dislocation tensor G

By $(2.8)_1$, $\mathrm{Curl}\,\mathbf{F}^p = \mathbf{0}$ when the plastic strain is *compatible* (the gradient of a vector field); $\mathrm{Curl}\,\mathbf{F}^p$ 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*,

$$\mathbf{b}^p(\partial S_\mathrm{R}) \equiv \int_{\partial S_\mathrm{R}} \mathbf{F}^p\,\mathrm{d}\mathbf{X} = \int_{S_\mathrm{R}} (\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T}\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R}. \tag{4.1}$$

For a single crystal the microscopic structure is a lattice and, since the vector $(\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T}\mathbf{n}_\mathrm{R}$ lies in the *lattice configuration*, one might associate $(\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T}\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R}$ with the Burgers vector corresponding to the boundary curve of a surface element with normal $\mathbf{n}_\mathrm{R}$, but that would be incorrect, as the surface element $\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R}$ lies in the *reference configuration* rather than in the lattice configuration. This is easily rectified. By $(3.9)_2$, $\mathbf{n}\,dA = J^p\mathbf{F}^{p-\mathrm{T}}\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R}$ is the surface element in the lattice configuration from which $\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R}$ convects; thus, formally,

$$(\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T}\mathbf{n}_\mathrm{R}\,\mathrm{d}A_\mathrm{R} = \frac{1}{J^p}(\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T}\mathbf{F}^{p\mathrm{T}}\mathbf{n}\,\mathrm{d}A \tag{4.2}$$

with $\mathbf{n}\,\mathrm{d}A$ the surface element in the lattice configuration, so that $(1/J^p)(\mathbf{F}^p\,\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T}\mathbf{n}\,\mathrm{d}A$ is the *local Burgers vector* corresponding to the "boundary curve" of the surface element $\mathbf{n}\,\mathrm{d}A$ in the *lattice configuration*. Thus, for

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

$\mathbf{G}^{p\mathrm{T}}\mathbf{n}$ 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 $\mathbf{n}$.

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

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

$(\mathbf{F}^{e-1} = (\mathbf{F}^e)^{-1})$. As before, $\mathrm{curl}\,\mathbf{F}^{e-1} = \mathbf{0}$ when $\mathbf{F}^e$ is compatible; $\mathrm{curl}\,\mathbf{F}^{e-1}$ therefore provides a measure of the local incompatibility of the structural deformation. Arguing as in the steps leading to (4.3), we may use $(3.10)_2$, again formally, to conclude that

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

Thus, by (4.4), for

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

$\mathbf{G}^{e\mathrm{T}}\mathbf{n}$ 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 $\mathbf{n}$. The fields $\mathbf{G}^{p\mathrm{T}}\mathbf{n}$ and $\mathbf{G}^{e\mathrm{T}}\mathbf{n}$ purportedly characterize the same Burgers vector. To reconcile this, note that, if $\bar{S}$ convects from S_R, then

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

so that $\mathbf{b}^e(\partial\bar{S}) = \mathbf{b}^p(\partial S_\mathrm{R})$. Therefore, by (3.8),

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

and, as $\bar{S}$ is arbitrary, $(\mathrm{Curl}\,\mathbf{F}^p)^\mathrm{T} = J(\mathrm{curl}\,\mathbf{F}^{e-1})^\mathrm{T}\mathbf{F}^{-\mathrm{T}}$.

Finally, since $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$ and $J = J^eJ^p$, we arrive at our main result: *The tensor fields* $\mathbf{G}^p$ *and* $\mathbf{G}^e$ *coincide. We refer to*

$$\mathbf{G} = \frac{1}{J^p}\mathbf{F}^p\,\mathrm{Curl}\,\mathbf{F}^p = J^e\mathbf{F}^{e-1}\mathrm{curl}\,\mathbf{F}^{e-1} \tag{4.5}$$

as the geometric dislocation tensor. Identity (4.5), our *main result*, is central to most of what follows. Reiterating, $\mathbf{G}^\mathrm{T}\mathbf{n}$ represents the (local) *Burgers vector* in the microstructural configuration — per unit area in that configuration — for the plane Π with unit normal $\mathbf{n}$; or in more physical terms, the local Burgers vector, per unit area, for those dislocation lines piercing Π. Here and in what follows, *we refer to* $\mathbf{G}^\mathrm{T}\mathbf{n}$ *as the Burgers vector even when the microstructural configuration does not represent a single crystal.*

An important consequence of (4.5) is that arguments regarding $\mathbf{G}$ are invariant under the replacement of the field $\mathbf{F}^p$ by the field $\mathbf{F}^{e-1}$ provided operations in the reference configuration are replaced by analogous operations in the deformed configuration.

5. Canonical decompositions of the geometric dislocation tensor

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 $\mathbf{l}$ is a *unit vector*.

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

$$\mathbf{G} = \mathbf{l}\otimes\mathbf{g} \quad \textit{with } \mathbf{g} \textit{ perpendicular to } \mathbf{l}, \tag{5.1}$$

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

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

$$\mathbf{G}=\mathbf{l}\otimes\mathbf{h} \quad \textit{with } \mathbf{h} \textit{ parallel to } \mathbf{l}, \tag{5.2}$$

so that $\mathbf{G}^{\mathrm{T}}\mathbf{l}=\mathbf{h}$, the Burgers vector for the plane $\mathbf{l}^{\perp}$, is perpendicular to $\mathbf{l}^{\perp}$. In this case $\mathbf{h}$ is termed the *principal Burgers vector* and $\mathbf{l}$ 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 $\mathbf{G}^{\mathrm{T}}\mathbf{n}$ 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 $\mathbf{G}^{\mathrm{T}}\mathbf{n}$ is always perpendicular to the plane $\mathbf{n}^{\perp}$.

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

Our next result gives canonical decompositions of $\mathbf{G}$ into "pure tensors" of the above form. *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* $\{\mathbf{l}_1,\mathbf{l}_2,\mathbf{l}_3\}$, *and vectors* $\{\mathbf{g}_1,\mathbf{g}_2,\mathbf{g}_3\}$ *with* $\mathbf{g}_i$ perpendicular *to* $\mathbf{l}_i$ *such that*

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

(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* $\{\mathbf{l}_1,\mathbf{l}_2,\mathbf{l}_3\}$, *and vectors* $\{\mathbf{h}_1,\mathbf{h}_2,\mathbf{h}_3\}$ *with* $\mathbf{h}_i$ *parallel to* $\mathbf{l}_i$ *such that*

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

(The orthonormal basis $\{\mathbf{l}_1,\mathbf{l}_2,\mathbf{l}_3\}$ in (i) is generally different from that in (ii).)

The verification of these decompositions is not difficult. Consequences of standard results are that $\mathbf{G}$ may be written in the form $\mathbf{G}=\varphi\mathbf{1}+\mathbf{G}_0$ with $\operatorname{tr}\mathbf{G}_0=0$. Further, there are scalars $\{\kappa_1,\kappa_2,\kappa_3\}$ and an orthonormal basis $\{\mathbf{l}_1,\mathbf{l}_2,\mathbf{l}_3\}$ such that $\operatorname{sym}\mathbf{G}_0=2\operatorname{sym}(\kappa_3\mathbb{N}_{12}+\kappa_2\mathbb{N}_{31}+\kappa_1\mathbb{N}_{23})$ with $\mathbb{N}_{ij}=\mathbf{l}_i\otimes\mathbf{l}_j$. (This is simply the decomposition of a deviatoric "strain-tensor" into simple shears on mutually orthogonal planes; cf., e.g., Gurtin, 1972, p. 36.) Further, given this decomposition, there are scalars $\{\zeta_1,\zeta_2,\zeta_3\}$ such that $\operatorname{skw}\mathbf{G}_0=-2\operatorname{skw}(\zeta_3\mathbb{N}_{12}+\zeta_2\mathbb{N}_{31}+\zeta_1\mathbb{N}_{23})$. Thus, letting $\mathbf{g}_1=(\kappa_3-\zeta_3)\mathbf{l}_2+(\kappa_2+\zeta_2)\mathbf{l}_3$, $\mathbf{g}_2=\ldots$, $\mathbf{g}_3=\ldots$ (with $\mathbf{g}_2$ and $\mathbf{g}_3$ obtained by cyclic permutation of the indices), we find that $\mathbf{G}_0=\sum_{i=1}^{3}\mathbf{l}_i\otimes\mathbf{g}_i$, which implies (5.3), since $\mathbf{G}_0=\operatorname{sym}\mathbf{G}_0+\operatorname{skw}\mathbf{G}_0$. Finally, there are an orthonormal basis $\{\mathbf{l}_1,\mathbf{l}_2,\mathbf{l}_3\}$, scalars $\{\lambda_1,\lambda_2,\lambda_3\}$, and a vector $\boldsymbol{\xi}$ such that $\operatorname{sym}\mathbf{G}=\sum_{i=1}^{3}\lambda_i\mathbf{l}_i\otimes\mathbf{l}_i$ with $\operatorname{skw}\mathbf{G}=\boldsymbol{\xi}\times$, which yields (5.4).

Consequences of this argument are the identities

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

By (3.14), for the special case in which $\mathbf{F}^p$ is a dilatation, $\mathbf{G}$ is an axial edge-tensor:

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

More generally, as a consequence of (2.8) we have a second canonical decomposition of $\mathbf{G}$: *Consider the decomposition* $\mathbf{F}^p = \lambda^{-1}\mathbf{F}_0^p$, $\det\mathbf{F}_0^p = 1$, *of* $\mathbf{F}^p$ *into isochoric and dilatational parts* (cf. (3.16)). *Then*

$$\mathbf{G} = \lambda\mathbf{G}_0 - \mathbf{F}_0^p(\nabla\lambda\times)\mathbf{F}_0^{p\mathrm{T}}, \ \mathbf{G}_0 = \mathbf{F}_0^p \operatorname{Curl}\mathbf{F}_0^p, \tag{5.7}$$

rendering $\mathbf{G}_0$ *the geometric dislocation tensor for the isochoric part of* $\mathbf{F}^p$.

6. G described relative to the reference and deformed configurations

$\mathbf{G}$ has a referential counterpart that may be obtained by transforming the vector $\mathbf{G}^{\mathrm{T}}\mathbf{n}\,dA$ to the reference configuration by premultiplication by $\mathbf{F}^{p-1}$ and then converting $\mathbf{n}\,dA$ to the referential surface element $\mathbf{n}_{\mathrm{R}}\,\mathrm{d}A_{\mathrm{R}}$ using $(3.9)_2$; the result is

$$\mathbf{G}_{\mathrm{R}} = J^p\mathbf{F}^{p-1}\mathbf{G}\mathbf{F}^{p-\mathrm{T}} = (\operatorname{Curl}\mathbf{F}^p)\mathbf{F}^{p-\mathrm{T}}, \tag{6.1}$$

$\mathbf{G}_{\mathrm{R}}^{\mathrm{T}}\mathbf{n}_{\mathrm{R}}$ gives the Burgers vector transported back to — and measured per unit area in — the reference configuration, $\mathbf{n}_{\mathrm{R}}\,\mathrm{d}A_{\mathrm{R}}$ being the relevant surface element. Similarly, transforming $\mathbf{G}^{\mathrm{T}}\mathbf{n}\,dA$ to the deformed configuration by premultiplication by $\mathbf{F}^e$ and then converting $\mathbf{n}\,dA$ to the deformed surface element $\bar{\mathbf{n}}\,\mathrm{d}\bar{A}$ using $(3.10)_2$ results in the tensor field

$$\bar{\mathbf{G}} = \frac{1}{J^e}\mathbf{F}^e\mathbf{G}\mathbf{F}^{e\mathrm{T}} = (\operatorname{curl}\mathbf{F}^{e-1})\mathbf{F}^{e\mathrm{T}}, \tag{6.2}$$

$\bar{\mathbf{G}}^{\mathrm{T}}\bar{\mathbf{n}}$ gives the Burgers vector convected to — and measured per unit area in — the deformed configuration, $\bar{\mathbf{n}}\,\mathrm{d}\bar{A}$ being the relevant surface element. $\mathbf{G}_{\mathrm{R}}$ and $\bar{\mathbf{G}}$ represent the geometric dislocation tensor $\mathbf{G}$ referred, respectively, to the reference and deformed configurations. Note that $\bar{\mathbf{G}} = \mathbf{G}_{\mathrm{Kr}}^e$ (cf. (1.3)).

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

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

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

$$\mathbf{G}^* = J^{e*}(\mathbf{F}^{e*})^{-1}\operatorname{curl}((\mathbf{F}^{e*})^{-1}) = \frac{1}{J^{p*}}\mathbf{F}^{p*}\operatorname{Curl}\mathbf{F}^{p*},$$
$$\mathbf{G}_{\mathrm{R}}^* = (\operatorname{Curl}\mathbf{F}^{p*})(\mathbf{F}^{p*})^{-\mathrm{T}}, \quad \bar{\mathbf{G}}^* = \operatorname{curl}((\mathbf{F}^{e*})^{-1})(\mathbf{F}^{e*})^{\mathrm{T}}. \tag{6.4}$$

By $(2.8)_2$, $\mathrm{Curl}(\mathbf{M}\mathbf{F}^p) = (\mathrm{Curl}\,\mathbf{F}^p)\mathbf{M}^{\mathrm{T}}$ and $\mathrm{curl}((\mathbf{F}^e\mathbf{M}^{-1})^{-1}) = (\mathrm{curl}\,\mathbf{F}^{e-1})\mathbf{M}^{\mathrm{T}}$; we therefore have the following transformation law for the geometric dislocation tensor under a homogeneous transformation of the microstructural configuration:

$$\mathbf{G}^* = (\det \mathbf{M})^{-1}\mathbf{M}\mathbf{G}\mathbf{M}^{\mathrm{T}}. \tag{6.5}$$

On the other hand, $\mathbf{G}_{\mathrm{R}}^* = \mathbf{G}_{\mathrm{R}}$ and $\bar{\mathbf{G}}^* = \bar{\mathbf{G}}$, 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 $\mathbf{R}^e$, and the lattice as it would appear to an observer is simply the lattice as framed in the microstructural configuration rotated via $\mathbf{R}^e$. The tensor

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

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 $\mathbf{x}_0$ in the deformed configuration. With this in mind, let $\mathbf{R}_0^e$ denote the lattice rotation at $\mathbf{x}_0$, so that

$$\mathbf{Q}^e = \mathbf{R}^e\mathbf{R}_0^{e\mathrm{T}}$$

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

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

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

7. Rigid-plastic materials

7.1. *Euler-angle representation of* $\mathbf{G}$

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 $\mathbf{G}$ in terms of gradients of Euler angles. This is the central objective of this section.

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

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

a definition that renders $\mathbf{Z}(\vartheta) = \exp(\vartheta\mathbf{A})$ the unique solution of the initial-value problem

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

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

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

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

$$\frac{\mathrm{d}\mathbf{Q}}{\mathrm{d}\vartheta} = (\mathbf{e}\times)\,\mathbf{Q}, \quad \frac{\mathrm{d}\mathbf{Q}^{\mathrm{T}}}{\mathrm{d}\vartheta} = -(\mathbf{e}\times)\,\mathbf{Q}^{\mathrm{T}}. \tag{7.4}$$

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

A representation of a rotation $\mathbf{R}$ in terms of *Euler angles* is a decomposition of $\mathbf{R}$ into the product of three rotations

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

of angles ϑ_i about unit vectors $\mathbf{c}_i$. The standard Euler-angle representation is obtained by choosing $\mathbf{c}_1 = \mathbf{c}_3 = \mathbf{k}$ and $\mathbf{c}_2 = \mathbf{i}$, with $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ 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

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

Any rotation may be represented in the standard form (7.6). (Cf., e.g., Synge (1960) and Kocks et al. (1998) for discussions of this and other rotation-representations common in mechanics and materials science.)

It is most convenient to work with the geometric dislocation tensor

$$\bar{\mathbf{G}} = \mathbf{R}^{e}\mathbf{G}\mathbf{R}^{e\mathrm{T}} = (\operatorname{curl} \mathbf{R}^{e\mathrm{T}})\mathbf{R}^{e\mathrm{T}}$$

(cf. (6.6)) referred to the deformed configuration. Consider the Euler-angle decomposition

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

where the $\mathbf{c}_i$ are *constant* unit vectors (with $\mathbf{c}_1$ microstructural). Before proceeding with the calculation of $\bar{\mathbf{G}}$, note that since $\mathbf{c}_1$ is the axis of the initial rotation $\mathbf{Q}_1$, $\mathbf{Q}_3\mathbf{Q}_2\mathbf{Q}_1\mathbf{c}_1 = \mathbf{Q}_3\mathbf{Q}_2\mathbf{c}_1$ represents $\mathbf{c}_1$ convected to the deformed configuration; and, since the rotation $\mathbf{Q}_2$ follows $\mathbf{Q}_1$, $\mathbf{Q}_3\mathbf{Q}_2\mathbf{c}_2 = \mathbf{Q}_3\mathbf{c}_2$ represents the convected value of $\mathbf{c}_2$. The unit vectors

$$\bar{\mathbf{c}}_1 = \mathbf{Q}_3\mathbf{Q}_2\mathbf{c}_1, \quad \bar{\mathbf{c}}_2 = \mathbf{Q}_3\mathbf{c}_2, \quad \bar{\mathbf{c}}_3 = \mathbf{c}_3$$

therefore represent the vectors $\mathbf{c}_i$ convected to the deformed configuration.

To calculate $\bar{\mathbf{G}}$, note that, by (2.9), (2.11), and (7.4), for $\mathbf{B}$ a rotation,

$$\begin{aligned}\operatorname{curl}(\mathbf{Q}_i^{\mathrm{T}}\mathbf{B}^{\mathrm{T}}) &= (\operatorname{curl} \mathbf{B}^{\mathrm{T}})\mathbf{Q}_i + (\operatorname{grad} \vartheta_i\times)\mathbf{B}(\mathbf{c}_i\times)\mathbf{Q}_i,\\ &= (\operatorname{curl} \mathbf{B}^{\mathrm{T}})\mathbf{Q}_i + (\operatorname{grad} \vartheta_i\times)\{(\mathbf{B}\mathbf{c}_i)\times\}\mathbf{B}\mathbf{Q}_i.\end{aligned} \tag{7.7}$$

Applying (7.7) with $i = 1$ and $\mathbf{B} = \mathbf{Q}_3\mathbf{Q}_2$ yields

$$\operatorname{curl} \mathbf{R}^{e\mathrm{T}} = \{\operatorname{curl}(\mathbf{Q}_2^{\mathrm{T}}\mathbf{Q}_3^{\mathrm{T}})\}\mathbf{Q}_1 + (\operatorname{grad} \vartheta_1\times)\{(\mathbf{Q}_3\mathbf{Q}_2\mathbf{c}_1)\times\}\mathbf{Q}_3\mathbf{Q}_2\mathbf{Q}_1.$$

Two more applications of (7.7), first to $\mathrm{curl}(\mathbf{Q}_2^{\mathrm{T}}\mathbf{Q}_3^{\mathrm{T}})$ and then to $\mathrm{curl}(\mathbf{Q}_3^{\mathrm{T}})$, leads to the expression

$$\mathrm{curl}\,\mathbf{R}^{e\mathrm{T}} = \{(\mathrm{grad}\,\vartheta_3\times)(\bar{\mathbf{c}}_3\times) + (\mathrm{grad}\,\vartheta_2\times)(\bar{\mathbf{c}}_2\times) + (\mathrm{grad}\,\vartheta_1\times)(\bar{\mathbf{c}}_1\times)\}\mathbf{R}^e.$$

Thus, in view of (2.7), *when represented in terms of Euler angles, the geometric dislocation tensor — referred to the deformed configuration — has the form*

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

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

7.2. Infinitesimal rotations. Nye's relation

The power series expansion (7.1) of $\mathbf{R}^e = \exp(\boldsymbol{\theta}\times)$, $\boldsymbol{\theta} = \vartheta\mathbf{e}$, yields the formal approximation

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

for small rotation-angles ϑ. The tensor field $\mathbf{W}^e$ represents the *infinitesimal rotation* and its axial vector $\boldsymbol{\theta}$ gives the *infinitesimal vector angle* of rotation. Consistent with (7.9), we approximate the geometric dislocation tensor $\mathbf{G} = \mathbf{R}^{e\mathrm{T}}\,\mathrm{curl}\,\mathbf{R}^{e\mathrm{T}}$ by the tensor field $\mathbf{G}_{\mathrm{inf}} = -\mathrm{curl}\,\mathbf{W}^e = -\mathrm{curl}(\boldsymbol{\theta}\times)$. Since $\mathrm{curl}(\mathbf{p}\times) = (\mathrm{div}\,\mathbf{p})\mathbf{1} - \mathrm{grad}\,\mathbf{p}$, this yields *Nye's relation* (1953)

$$\mathbf{G}_{\mathrm{inf}} = \mathbf{N} - (\mathrm{tr}\,\mathbf{N})\mathbf{1}, \quad \mathbf{N} = \mathrm{grad}\,\boldsymbol{\theta}. \tag{7.10}$$

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 normal $\mathbf{n}$. By $(3.9)_1$ and (3.10), $\mathbf{n}$, which is *constant*, convects from a *field* $\mathbf{n}_{\mathrm{R}}(\mathbf{X})$ of unit normals in the reference configuration and to a *field* $\bar{\mathbf{n}}(\mathbf{x})$ of unit normals in the deformed configuration, where

$$\begin{aligned}&\lambda_{\mathrm{R}}\mathbf{n}_{\mathrm{R}} = \mathbf{F}^{p\mathrm{T}}\mathbf{n}, \ \ \lambda_{\mathrm{R}} = |\mathbf{F}^{p\mathrm{T}}\mathbf{n}|,\\ &\bar{\lambda}\bar{\mathbf{n}} = \mathbf{F}^{e-\mathrm{T}}\mathbf{n}, \ \ \bar{\lambda} = |\mathbf{F}^{e-\mathrm{T}}\mathbf{n}|\end{aligned} \tag{8.1}$$

an interesting question is whether the field $\bar{\mathbf{n}}$, 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* $\mathbf{n}\cdot\mathbf{G}\mathbf{n}$ *measures the distortion of the microstructural plane* Π.

Let Π denote a *fixed plane* in the microstructural configuration, with $\mathbf{n}$ its unit normal. We say that Π is *globally undistorted* if the unit-normal field $\bar{\mathbf{n}}(\mathbf{x})$ to which

$\mathbf{n}$ convects is a normal field for a family of smooth surfaces in the deformed body $\bar{B}$; that is, if, given any $\mathbf{x}$ in $\bar{B}$: (i) $\mathbf{x}$ is contained in a single surface $\bar{S}$ of the family; and (ii) $\bar{\mathbf{n}}(\mathbf{x})$ is normal to $\bar{S}$ at $\mathbf{x}$. This notion could equally well have been phrased with respect to the reference configuration: there is a family of smooth surfaces in $\bar{B}$ for which $\bar{\mathbf{n}}$ is a normal field if and only if there is a family of smooth surfaces in B_{R} for which $\mathbf{n}_{\mathrm{R}}$ is a normal field.

We now show that: *a necessary and sufficient condition that Π be globally undistorted is that $\mathbf{n}\cdot\mathbf{G}\mathbf{n}$ vanish at each point of the body.*

To establish this assertion, note first that, by (8.1),

$$(\mathbf{F}^{p\mathrm{T}}\mathbf{n})\cdot\mathrm{Curl}(\mathbf{F}^{p\mathrm{T}}\mathbf{n}) = \lambda_{\mathrm{R}}\mathbf{n}_{\mathrm{R}}\cdot[\lambda_{\mathrm{R}}\,\mathrm{Curl}\,\mathbf{n}_{\mathrm{R}} + (\nabla\lambda_{\mathrm{R}})\times\mathbf{n}_{\mathrm{R}}] = \lambda_{\mathrm{R}}^2\mathbf{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\mathbf{n}_{\mathrm{R}}$$

and

$$(\mathbf{F}^{e-\mathrm{T}}\mathbf{n})\cdot\mathrm{curl}(\mathbf{F}^{e-\mathrm{T}}\mathbf{n}) = \bar{\lambda}^{2}\,\bar{\mathbf{n}}\cdot\mathrm{curl}\,\bar{\mathbf{n}}.$$

Therefore (4.5) yields the interesting relations

$$\mathbf{n}\cdot\mathbf{G}\mathbf{n} = J^e\bar{\lambda}^{2}\,\bar{\mathbf{n}}\cdot\mathrm{curl}\,\bar{\mathbf{n}} = \frac{\lambda_{\mathrm{R}}^2}{J^p}\,\mathbf{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\mathbf{n}_{\mathrm{R}}. \tag{8.2}$$

Thus a necessary and sufficient condition that $\mathbf{n}\cdot\mathbf{G}\mathbf{n}$ vanish at a given point is that $\bar{\mathbf{n}}\cdot\mathrm{curl}\,\bar{\mathbf{n}}=0$ (*or equivalently*, $\mathbf{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\mathbf{n}_{\mathrm{R}}=0$). Roughly speaking, $\bar{\mathbf{n}}\cdot\mathrm{curl}\,\bar{\mathbf{n}}$ represents the twist of the vector field $\bar{\mathbf{n}}$ about itself, and similarly for $\mathbf{n}_{\mathrm{R}}\cdot\mathrm{Curl}\,\mathbf{n}_{\mathrm{R}}$. Note that for a *rigid-plastic material*,

$$\mathbf{n}\cdot\mathbf{G}\mathbf{n} = \bar{\mathbf{n}}\cdot\mathrm{curl}\,\bar{\mathbf{n}}.$$

Finally, a classical theorem of Frobenius (Choquet-Bruhat and DeWitt-Morette, 1977, p. 235) asserts that a necessary and sufficient condition that $\bar{\mathbf{n}}(\mathbf{x})$ be a normal field for a family of smooth surfaces in $\bar{B}$ is that $\bar{\mathbf{n}}\cdot\mathrm{curl}\,\bar{\mathbf{n}}=0$ everywhere in $\bar{B}$; thus, by (8.2), Π is globally undistorted if and only if $\mathbf{n}\cdot\mathbf{G}\mathbf{n}\equiv 0$.

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

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

$$\bar{\mathbf{n}}(\mathbf{z}(0)) = \bar{\mathbf{m}}(\mathbf{z}(0)),\quad \left[\frac{\mathrm{d}}{\mathrm{d}\sigma}\bar{\mathbf{n}}(\mathbf{z}(\sigma))\right]_{\sigma=0} = \left[\frac{\mathrm{d}}{\mathrm{d}\sigma}\bar{\mathbf{m}}(\mathbf{z}(\sigma))\right]_{\sigma=0}. \tag{8.3}$$

It then follows that: *a necessary and sufficient condition that Π be locally undistorted at a given point is that $\mathbf{n}\cdot\mathbf{G}\mathbf{n}$ vanish at that point.*

The proof of this assertion, which is technical and beyond the scope of the present paper, is given by Cermelli and Gurtin (2000, Section 13.1).

9. Strict plane strain

9.1. Principal Burgers vector g

We now discuss the form of the geometric dislocation tensor for strict plane strain as defined in Section 3.5. We begin with two useful identities. Let $\mathbf{T}$ be a planar tensor field. Then

$$\operatorname{Curl}\mathbf{T} = \mathbf{e}\otimes\mathbf{q}, \quad \mathbf{q} = (\operatorname{Curl}\mathbf{T})^{\mathrm{T}}\mathbf{e} \tag{9.1}$$

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

$$\mathbf{T}(\mathbf{e}\times) = \det\mathbf{T}(\mathbf{e}\times)\mathbf{T}^{-\mathrm{T}}. \tag{9.2}$$

To verify (9.1), note that, for $\mathbf{c}$ a constant vector, $\mathbf{T}^{\mathrm{T}}\mathbf{c} = \mathbf{p} + c_3\mathbf{e}$ with $\mathbf{p}$ planar; thus, since $\operatorname{Curl}\mathbf{p}$ is parallel to $\mathbf{e}$, $\mathbb{P}(\mathbf{e})(\operatorname{Curl}\mathbf{T})\mathbf{c} = \mathbb{P}(\mathbf{e})\operatorname{Curl}(\mathbf{T}^{\mathrm{T}}\mathbf{c}) = \mathbb{P}(\mathbf{e})\operatorname{Curl}\mathbf{p} = \mathbf{0}$. But $\mathbf{c}$ is arbitrary, thus $\mathbb{P}(\mathbf{e})\operatorname{Curl}\mathbf{T} = \mathbf{0}$ and, since $\mathbb{P}(\mathbf{e}) = \mathbf{1} - \mathbf{e}\otimes\mathbf{e}$, $\operatorname{Curl}\mathbf{T} = \mathbf{e}\otimes(\operatorname{Curl}\mathbf{T})^{\mathrm{T}}\mathbf{e} = \mathbf{e}\otimes\mathbf{q}$. Further, $\mathbf{q}\cdot\mathbf{e} = \mathbf{e}\cdot(\operatorname{Curl}\mathbf{T})\mathbf{e} = \mathbf{e}\cdot\operatorname{Curl}(\mathbf{T}^{\mathrm{T}}\mathbf{e}) = \mathbf{e}\cdot\operatorname{Curl}\mathbf{e} = 0$ and $\mathbf{q}$ is planar. This proves the first assertion. Since $\mathbf{T}$ is planar, the second, (9.2), follows from (2.11): $\mathbf{T}(\mathbf{e}\times) = \det\mathbf{T}\,\{(\mathbf{T}^{-\mathrm{T}}\mathbf{e})\times\}\mathbf{T}^{-\mathrm{T}} = \det\mathbf{T}(\mathbf{e}\times)\mathbf{T}^{-\mathrm{T}}$.

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

$$\mathbf{G} = \frac{1}{J^p}\mathbf{F}^p\operatorname{Curl}\mathbf{F}^p = \frac{1}{J^p}(\mathbf{F}^p\mathbf{e})\otimes(\operatorname{Curl}\mathbf{F}^p)^{\mathrm{T}}\mathbf{e} = \mathbf{e}\otimes\left(\frac{1}{J^p}\operatorname{Curl}\mathbf{F}^p\right)^{\mathrm{T}}\mathbf{e},$$

or equivalently,

$$\mathbf{G} = J^e\mathbf{F}^{e-1}\operatorname{curl}\mathbf{F}^{e-1} = \mathbf{e}\otimes(J^e\operatorname{curl}\mathbf{F}^{e-1})^{\mathrm{T}}\mathbf{e}.$$

The geometric dislocation tensor is therefore a pure edge-tensor

$$\mathbf{G} = \mathbf{e}\otimes\mathbf{g} \tag{9.3}$$

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

$$\mathbf{g} = J^e(\operatorname{curl}\mathbf{F}^{e-1})^{\mathrm{T}}\mathbf{e} = \frac{1}{J^p}(\operatorname{Curl}\mathbf{F}^p)^{\mathrm{T}}\mathbf{e}. \tag{9.4}$$

(A vector field $\mathbf{u}$ is *planar* if $\mathbf{u}$ is independent of X_3 (or equivalently, x_3) and satisfies $\mathbf{u}\cdot\mathbf{e}=0$, so that $\operatorname{Curl}\mathbf{u}$ *is parallel to* $\mathbf{e}$.) Thus, $\mathbf{g}$ 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 $\mathbf{n}\cdot\mathbf{G}\mathbf{n} = (\mathbf{g}\cdot\mathbf{n})(\mathbf{e}\cdot\mathbf{n})$; we may therefore conclude from the results of Section 8 that: *a microstructural plane parallel to* $\mathbf{e}$ *is globally undistorted*; *a microstructural plane parallel to* $\mathbf{g}$ *at some point is there locally undistorted.*

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

$$\mathbf{G}_{\mathrm{R}} = \mathbf{e}\otimes\mathbf{g}_{\mathrm{R}}, \quad \mathbf{g}_{\mathrm{R}} = J^p\mathbf{F}^{p-1}\mathbf{g}, \tag{9.5}$$

when referred to the reference configuration, and by

$$\bar{\mathbf{G}} = \mathbf{e}\otimes\bar{\mathbf{g}}, \;\; \bar{\mathbf{g}} = \frac{1}{J^e}\mathbf{F}^e\mathbf{g}, \tag{9.6}$$

when referred to the deformed configuration.

The rotation and stretch tensors defined by the polar decomposition (3.5) of $\mathbf{F}^e$ are planar tensor fields; the lattice rotation $\mathbf{R}^e$ may therefore be expressed in the form

$$\mathbf{R}^e = \mathbf{R}^e(\vartheta^e) \tag{9.7}$$

with ϑ^e an angle that measures the lattice rotation in a counterclockwise direction about $\mathbf{e}$. Applying identities (2.9) and $(7.4)_3$ to $\mathrm{Curl}\,\mathbf{F}^{e-1}$ with $\mathbf{F}^e = \mathbf{V}^e\mathbf{R}^e$,

$$\begin{aligned}\mathrm{curl}\,\mathbf{F}^{e-1} &= (\mathrm{curl}\,\mathbf{V}^{e-1})\mathbf{R}^e + (\mathrm{grad}\,\vartheta^e\times)\left(\frac{\mathrm{d}\mathbf{R}^{e\mathrm{T}}}{\mathrm{d}\vartheta^e}\mathbf{V}^{e-1}\right)^{\mathrm{T}} \\ &= (\mathrm{curl}\,\mathbf{V}^{e-1})\mathbf{R}^e - (\mathrm{grad}\,\vartheta^e\times)[(\mathbf{e}\times)\mathbf{F}^{e-1}]^{\mathrm{T}},\end{aligned}$$

so that, by (9.2) with $\mathbf{T} = \mathbf{F}^{e-1}$,

$$\begin{aligned}\mathbf{g} &= J^e\{\mathbf{R}^{e\mathrm{T}}(\mathrm{curl}\,\mathbf{V}^{e-1})^{\mathrm{T}}\mathbf{e} - (\mathbf{e}\times)\mathbf{F}^{e-1}(\mathbf{e}\times\mathrm{grad}\,\vartheta^e)\} \\ &= J^e\mathbf{R}^{e\mathrm{T}}(\mathrm{curl}\,\mathbf{V}^{e-1})^{\mathrm{T}}\mathbf{e} - (\mathbf{e}\times)(\mathbf{e}\times)\mathbf{F}^{e\mathrm{T}}\mathrm{grad}\,\vartheta^e.\end{aligned}$$

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

$$\mathbf{g} = J^e\,\mathbf{R}^{e\mathrm{T}}(\mathrm{curl}\,\mathbf{V}^{e-1})^{\mathrm{T}}\mathbf{e} + \mathbf{F}^{e\mathrm{T}}\,\mathrm{grad}\,\vartheta^e. \tag{9.8}$$

9.2. Rigid-plastic materials

By (9.6),

$$\bar{\mathbf{g}} = \mathbf{R}^e\mathbf{g} \tag{9.9}$$

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)). Since $\mathbf{V}^e = \mathbf{1}$, $\mathrm{curl}\,\mathbf{V}^{e-1} = \mathbf{0}$; relations (9.8) and (9.9) reduce to

$$\mathbf{g} = \mathbf{R}^{e\mathrm{T}}\,\mathrm{grad}\,\vartheta^e \quad \text{and} \quad \bar{\mathbf{g}} = \mathrm{grad}\,\vartheta^e; \tag{9.10}$$

$\bar{\mathbf{g}}$ is hence normal to surfaces $\vartheta^e = \text{constant}$ in the deformed configuration. 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. Relation $(9.10)_2$ shows that — granted strict plane strain — such layers are necessarily accompanied by geometrically necessary dislocations and, when sufficiently thin, should have Burgers vector approximately normal to the layer.

Under strict plane strain the underlying fields may be considered as functions of their position (x_1, x_2) in the cross-sectional plane $\mathscr{P}$. Consider, for the moment, a single crystal. Then $\bar{\mathbf{s}}^\alpha = \mathbf{R}^e\mathbf{s}^\alpha$ and $\bar{\mathbf{m}}^\alpha = \mathbf{R}^e\mathbf{m}^\alpha$ and for planar slip systems the family of deformed slip planes for α may be identified with the family of (smooth) deformed slip curves in $\mathscr{P}$ tangent to the field $\bar{\mathbf{s}}^\alpha$. By $(9.10)_2$, $\mathbf{s}^\alpha\cdot\mathbf{g} = \bar{\mathbf{s}}^\alpha\cdot\mathrm{grad}\,\vartheta^e$ *represents a curvature field for the deformed slip curves*. Similarly, $\mathbf{m}^\alpha\cdot\mathbf{g} = \bar{\mathbf{m}}^\alpha\cdot\mathrm{grad}\,\vartheta^e$ represents a curvature field for the family of smooth curves tangent to $\bar{\mathbf{m}}^\alpha$.

Returning to general rigid-plastic materials, $\mathbf{R}^{e\mathrm{T}}\,\mathrm{grad}\,\vartheta^e = \mathbf{F}^{p-\mathrm{T}}\nabla\vartheta^e$, since $\mathbf{F} = \mathbf{R}^e\mathbf{F}^p$ and $\mathbf{F}^{\mathrm{T}}\,\mathrm{grad}\,\vartheta^e = \nabla\vartheta^e$, and this yields the alternative relation

$$\mathbf{g} = \mathbf{F}^{p-\mathrm{T}}\,\nabla\vartheta^e. \tag{9.11}$$

In many situations of interest the structural strains are small in the sense that $\mathbf{V}^e \approx \mathbf{1}$, so that, formally, $\mathbf{V}^{e-1} \approx \mathbf{1}$, and $\operatorname{curl}\mathbf{V}^{e-1} \approx \mathbf{0}$. In this case the foregoing relations hold to within the same approximation.

10. Strict anti-plane shear

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

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

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

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

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

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

with γ^p and γ^e normal to $\mathbf{e}$. Then $J^e = 1$, $J^p = 1$, and, in addition, the decomposition $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$ yields $\gamma = \gamma^e + \gamma^p$. Since $\gamma = \nabla u$, $\operatorname{curl}\gamma = \mathbf{0}$; thus $\operatorname{curl}\gamma^p = -\operatorname{curl}\gamma^e$. (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 $(2.8)_5$, $\operatorname{curl}\mathbf{F}^p = (\operatorname{curl}\gamma^p) \otimes \mathbf{e}$. Moreover, since $\gamma \cdot \mathbf{e} = 0$, $\operatorname{curl}\gamma^p$ and $\operatorname{curl}\gamma^e$ are parallel to $\mathbf{e}$; thus $\operatorname{curl}\mathbf{F}^p = \mathbf{e} \otimes \operatorname{curl}\gamma^p$ with $\gamma^p \cdot \operatorname{curl}\gamma^p = 0$. Thus, since $\mathbf{G} = \mathbf{F}^p \operatorname{curl}\mathbf{F}^p$, *the geometric dislocation tensor is a pure screw-tensor*

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

with principal Burgers vector

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

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

11. Transport of geometrically necessary dislocations

11.1. Dislocation densities. Balance law for dislocations

We now show 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

$$\mathbf{l} \otimes \mathbf{b} \ldots \begin{cases} \mathbf{l} \perp \mathbf{b}, & \text{edge,} \\ \mathbf{l} = \mathbf{b}, & \text{screw} \end{cases} \tag{11.1}$$

with $\mathbf{l}$ and $\mathbf{b}$ microstructural *unit vectors.*[2] We refer to each such pair $\mathsf{d} = (\mathbf{l}, \mathbf{b})$ as a *dislocation dyad* with *Burgers direction* $\mathbf{b}$ and *line direction* $\mathbf{l}$. The scalar field

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

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

The vector fields

$$\mathbf{l}_{\mathrm{R}} = \mathbf{F}^{p\mathrm{T}}\mathbf{l}, \quad \mathbf{b}_{\mathrm{R}} = \mathbf{F}^{p\mathrm{T}}\mathbf{b}$$

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

$$(\mathrm{Curl}\,\mathbf{F}^p)\mathbf{b} = \mathrm{Curl}\,\mathbf{b}_{\mathrm{R}}, \quad (\mathrm{Curl}\,\mathbf{F}^p)\mathbf{l} = \mathrm{Curl}\,\mathbf{l}_{\mathrm{R}}, \tag{11.3}$$

if $J^p = 1$, then (4.5) leads to the simple expression $\rho = \mathbf{l}_{\mathrm{R}} \cdot \mathrm{Curl}\,\mathbf{b}_{\mathrm{R}}$; hence

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

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

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

Further, we may use (2.11) to conclude that $(\mathbf{F}^{p\mathrm{T}}\mathbf{l})\times = \mathbf{F}^{p-1}(\mathbf{l}\times)\mathbf{F}^{p-\mathrm{T}}$, and hence that

$$\mathbf{l}_{\mathrm{R}} \times \dot{\mathbf{b}}_{\mathrm{R}} = \{(\mathbf{F}^{p\mathrm{T}}\mathbf{l})\times\}\mathbf{F}^{p\mathrm{T}}\mathbf{L}^{p\mathrm{T}}\mathbf{b} = \mathbf{F}^{p-1}(\mathbf{l}\times)\mathbf{L}^{p\mathrm{T}}\mathbf{b}.$$

We therefore have the *balance law for dislocations*: *Granted* $J^p = 1$, *the dislocation density* $\rho = \rho(\mathbf{l}, \mathbf{b})$ *has the simple form* $\rho = \mathbf{l}_{\mathrm{R}} \cdot \mathrm{Curl}\,\mathbf{b}_{\mathrm{R}}$ *and evolves according to*

$$\dot{\rho} = -\mathrm{Div}\,\mathbf{q}_{\mathrm{R}} + \sigma_{\mathrm{R}} \tag{11.4}$$

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

$$\mathbf{q}_{\mathrm{R}} = \mathbf{F}^{p-1}(\mathbf{l} \times (\mathbf{L}^{p\mathrm{T}}\mathbf{b})), \;\; \sigma_{\mathrm{R}} = 2(\mathrm{sym}\,\mathbf{l} \otimes \mathbf{b}) \cdot (\mathbf{L}^p\mathbf{G}). \tag{11.5}$$

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

$$\mathbf{q}_{\mathrm{R}} = \mathbf{l}_{\mathrm{R}} \times \dot{\mathbf{b}}_{\mathrm{R}}, \quad \sigma_{\mathrm{R}} = \dot{\mathbf{l}}_{\mathrm{R}} \cdot \mathrm{Curl}\,\mathbf{b}_{\mathrm{R}} + \dot{\mathbf{b}}_{\mathrm{R}} \cdot \mathrm{Curl}\,\mathbf{l}_{\mathrm{R}}.$$

Further, for a single crystal, we may use (3.13) and (4.5) to conclude that

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

[2] 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 $\{1\,1\,1\}\langle 1\,1\,0\rangle$ slip systems in fcc crystals a canonical set of dyads consists of 6 pure screw directions with line directions in the $\langle 1\,1\,0\rangle$ directions and 12 pure edge directions whose line directions lie in $\langle 1\,1\,2\rangle$ directions and whose Burgers vectors lie along $\langle 1\,1\,0\rangle$. 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.

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

11.2. Properties of the dislocation flux

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

$$\mathbf{q}(\mathbf{l},\mathbf{b}) \stackrel{\text{def}}{=} \mathbf{F}^p \mathbf{q}_{\mathrm{R}}(\mathbf{l},\mathbf{b}) = (\mathbf{l}\times)\mathbf{L}^{p\mathrm{T}}\mathbf{b}, \tag{11.6}$$

which is $\mathbf{q}_{\mathrm{R}}$ convected to the microstructural configuration, lies in the plane $\mathbf{l}^\perp$. Moreover, plastic flow is always associated with a flux of dislocations — that is, $\mathbf{L}^p \neq \mathbf{0}$ if and only if $\mathbf{q}_{\mathrm{R}}(\mathbf{l},\mathbf{b}) \neq \mathbf{0}$ for some choice of $\mathbf{l}$ and $\mathbf{b}$ — and this is true even when $\mathbf{G} \equiv \mathbf{0}$, but in this case $\varrho \equiv 0$, $\sigma_{\mathrm{R}} \equiv 0$, and the flow is *equilibrated*: $\operatorname{Div}\mathbf{q}_{\mathrm{R}} = 0$. Further, *the dislocation fluxes determine* $\mathbf{L}^p$: for $\{\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3\}$ an arbitrarily chosen orthonormal basis and any choice of i and j, $i \neq j$, $\mathbf{e}_i \cdot \mathbf{L}^p\mathbf{e}_j = (\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{q}(\mathbf{e}_i,\mathbf{e}_i)$ and $\mathbf{e}_i \cdot \mathbf{L}^p\mathbf{e}_i = (\mathbf{e}_j \times \mathbf{e}_i) \cdot \mathbf{q}(\mathbf{e}_j,\mathbf{e}_i)$; the off-diagonal components of $\mathbf{L}^p$ are therefore determined by the screw-density fluxes $\mathbf{q}(\mathbf{e}_i,\mathbf{e}_i)$, the diagonal components by the edge-density fluxes $\mathbf{q}(\mathbf{e}_i,\mathbf{e}_j)$.

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

The microstructural flux $\mathbf{q}$ corresponding to $\mathbf{G}$ resolved on the dislocation system $\mathsf{d} = (\mathbf{l},\mathbf{b})$ 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 d of edge type. Consider first a single active slip system, so that $\mathbf{L}^p = v^\alpha(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)$. Our computation of Burgers vectors uses a right-hand screw-rule, and therefore the *natural line direction* $\mathbf{l}^\alpha$ *for edge dislocations* moving on this slip system is $\mathbf{l}^\alpha = \mathbf{m}^\alpha \times \mathbf{s}^\alpha$, 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 $\mathbf{m}^\alpha$ points) moving in the direction $\mathbf{s}^\alpha$ relative to material below the plane. The flux $\mathbf{q}$ of dislocations — as resolved on the system d — due to slip on α should have the following properties: (i) $\mathbf{q}$ should be orthogonal to the dislocation line and hence to $\mathbf{l}$, since the tangential motion of a dislocation line is irrelevant; (ii) $\mathbf{q}$ should lie in the slip plane and should hence be orthogonal to $\mathbf{m}^\alpha$; (iii) the magnitude of $\mathbf{q}$ should be $(v^\alpha\mathbf{s}^\alpha) \cdot \mathbf{b}$; (iv) for $\mathbf{l}$ the natural line direction for slip on α, the flux should be $(\mathbf{s}^\alpha \cdot \mathbf{b})\mathbf{s}^\alpha$. These conditions determine $\mathbf{q}$. Indeed, (i) and (ii) imply that $\mathbf{q}$ should lie on the line spanned by the unit vector $\mathbf{l} \times \mathbf{m}^\alpha$ and hence, by (iii), should have the form $\pm v^\alpha(\mathbf{s}^\alpha \cdot \mathbf{b})\mathbf{l} \times \mathbf{m}^\alpha$. Since $\mathbf{l}^\alpha = \mathbf{m}^\alpha \times \mathbf{s}^\alpha$, condition (iv) requires that we take the positive sign

$$\mathbf{q} = \nu^\alpha(\mathbf{s}^\alpha \cdot \mathbf{b})\,\mathbf{l} \times \mathbf{m}^\alpha = (\mathbf{l}\times)(\nu^\alpha\, \mathbb{S}^{\alpha\mathrm{T}})\mathbf{b}.$$

If we allow for the possibility of all slip systems being active, then we arrive at formula (11.6) for the dislocation flux as measured in the microstructural configuration.

11.3. Relations for $\dot{\mathbf{G}}$

In discussing geometrically necessary dislocations in single crystals it would seem useful to have available identities relating $\dot{\mathbf{G}}$ to the slips ν^α and their gradients. By (4.5),

$$\dot{\mathbf{G}} = \left(\overline{\frac{1}{J^p}\mathbf{F}^p}^{\,\cdot}\right) \operatorname{Curl} \mathbf{F}^p + \frac{1}{J^p}\mathbf{F}^p \operatorname{Curl} \dot{\mathbf{F}}^p, \tag{11.7}$$

while $(2.8)_2$ and (3.4) yield

$$\operatorname{Curl} \dot{\mathbf{F}}^p = (\operatorname{Curl} \mathbf{F}^p)\mathbf{L}^{p\mathrm{T}} + \operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p), \tag{11.8}$$

where $\operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p)$ is the Curl of $\mathbf{L}^p\mathbf{F}^p$ holding $\mathbf{F}^p$ fixed. Thus, by (3.4) and since $\dot{J}^p = J^p \operatorname{tr} \mathbf{L}^p$,

$$\dot{\mathbf{G}} = -(\operatorname{tr} \mathbf{L}^p)\mathbf{G} + \mathbf{L}^p\mathbf{G} + \mathbf{G}\mathbf{L}^{p\mathrm{T}} + \frac{1}{J^p}\mathbf{F}^p \operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p). \tag{11.9}$$

The term $\operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p)$ is, in general, complicated, but it does reduce when attention is restricted to *single crystals*. In that case $\mathbf{L}^p$ has the explicit form (3.13) and $\operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p)$ comes from computing $\operatorname{Curl}(\mathbf{L}^p\mathbf{F}^p) = \sum_{\alpha=1}^{A} \operatorname{Curl}\{\nu^\alpha\, \mathbb{S}^\alpha\mathbf{F}^p\}$ holding $\mathbf{F}^p$ fixed, or equivalently holding $\mathbb{S}^\alpha\mathbf{F}^p$ fixed for each α. Thus $(2.8)_3$, (2.11), and the fact that $J^p = 1$ yield $\mathbf{F}^p \operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p) = \sum_{\alpha=1}^{A} \mathbf{F}^p(\nabla\nu^\alpha\times)\mathbf{F}^{p\mathrm{T}}\,\mathbb{S}^{\alpha\mathrm{T}} = \sum_{\alpha=1}^{A}\{(\mathbf{F}^{p-\mathrm{T}}\nabla\nu^\alpha)\times\}\,\mathbb{S}^{\alpha\mathrm{T}}$.

Further, since $\nabla\nu^\alpha = \mathbf{F}^{\mathrm{T}} \operatorname{grad} \nu^\alpha$ and $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$,

$$\mathbf{F}^{p-\mathrm{T}}\nabla\nu^\alpha = \mathbf{F}^{e\mathrm{T}} \operatorname{grad} \nu^\alpha \stackrel{\mathrm{def}}{=} \nabla_{\mathrm{L}}\, \nu^\alpha, \tag{11.10}$$

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 (11.9) therefore takes the form

$$\dot{\mathbf{G}} = \sum_{\alpha=1}^{A} [\nu^\alpha\{\mathbb{S}^\alpha\mathbf{G} + \mathbf{G}\mathbb{S}^{\alpha\mathrm{T}}\} - \{\mathbf{m}^\alpha \times \nabla_{\mathrm{L}}\, \nu^\alpha\} \otimes \mathbf{s}^\alpha]. \tag{11.11}$$

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

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

Under strict plane strain $\mathbf{L}^p\mathbf{e} = \mathbf{L}^{p\mathrm{T}}\mathbf{e} = \mathbf{0}$ and $\mathbf{G} = \mathbf{e} \otimes \mathbf{g}$ with $\mathbf{e}$ constant; the analog of (11.9) is therefore

$$\dot{\mathbf{g}} = (\mathbf{L}^p - (\operatorname{tr} \mathbf{L}^p)\mathbf{1})\,\mathbf{g} + \frac{1}{J^p}[\operatorname{Curl}_{\mathbf{L}^p}(\mathbf{L}^p\mathbf{F}^p)]^{\mathrm{T}}\mathbf{e}. \tag{11.12}$$

Next, in view of (3.4) and the identity $\overline{\mathbf{T}^{-1}}^{\cdot} = -\mathbf{T}^{-1}\dot{\mathbf{T}}\mathbf{T}^{-1}$, it follows that $\overline{\mathbf{F}^{p-\mathrm{T}}}^{\cdot} = -\mathbf{L}^{p\mathrm{T}}\mathbf{F}^{p-\mathrm{T}}$. Thus for a rigid-plastic material an equivalent expression in terms of the elastic rotation angle follows upon differentiation of (9.11):

$$\dot{\mathbf{g}} = -\mathbf{L}^{p\mathrm{T}}\mathbf{g} + \nabla_{\mathrm{L}}\dot{\vartheta}^{e}. \tag{11.13}$$

The specialization to single crystals may be obtained by direct substitution of $\mathbf{G}=\mathbf{e}\otimes\mathbf{g}$ into (11.11):

$$\dot{\mathbf{g}} = \sum_{\alpha=1}^{A} [(\mathbf{g}\cdot\mathbf{m}^{\alpha})v^{\alpha} + (\mathbf{s}^{\alpha}\cdot\nabla_{\mathrm{L}}\, v^{\alpha})]\mathbf{s}^{\alpha}. \tag{11.14}$$

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

$$\dot{\mathbf{g}} = \sum_{\alpha=1}^{A} [(\mathbf{m}^{\alpha}\cdot\nabla_{\mathrm{L}}\,\vartheta^{e})v^{\alpha} + (\mathbf{s}^{\alpha}\cdot\nabla_{\mathrm{L}}\, v^{\alpha})]\mathbf{s}^{\alpha}. \tag{11.15}$$

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 $\mathbf{F}^{p}$ and $\nabla\mathbf{F}^{p}$ display this invariance.

Let $\mathbf{X}_0$ denote an arbitrarily prescribed material point. By a *compatible change in local reference* (at $\mathbf{X}_0$) we mean a smooth one-to-one mapping $\mathbf{Z}=\mathbf{Z}(\mathbf{X})$ of a neighborhood of $\mathbf{X}_0$ onto an open set in $\mathbb{R}^3$; the points $\mathbf{Z}$ then represent new labels for material points. We write $\hat{\nabla}$ for the gradient with respect to points $\mathbf{Z}$, leaving ∇ to denote the gradient with respect to $\mathbf{X}$. Writing $\mathbf{X}=\mathbf{X}(\mathbf{Z})$ for the inverse of the mapping $\mathbf{Z}=\mathbf{Z}(\mathbf{X})$, let $\mathbf{H}=\hat{\nabla}\mathbf{X}$ and assume that $\det\mathbf{H} > 0$.

When expressed relative to the new reference, a motion $\mathbf{x}=\mathbf{y}(\mathbf{X})$ and its gradient are given by

$$\mathbf{x} = \hat{\mathbf{y}}(\mathbf{Z}) = \mathbf{y}(\mathbf{X}(\mathbf{Z})), \quad \hat{\mathbf{F}} = \hat{\nabla}\hat{\mathbf{y}} = \mathbf{F}\mathbf{H}. \tag{12.1}$$

The structural transformation $\mathbf{F}^{e}$ 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 $\mathbf{F}^{e}$ be invariant under local changes in reference. On the other hand, by (12.1) and the decomposition $\mathbf{F}=\mathbf{F}^{e}\mathbf{F}^{p}$, the plastic strain $\hat{\mathbf{F}}^{p}$ relative to the new reference must, for consistency, satisfy

$$\hat{\mathbf{F}}^{p} = \mathbf{F}^{p}\mathbf{H}, \quad \hat{J}^{p} = (\det\mathbf{H})J^{p}. \tag{12.2}$$

A discussion of the geometric dislocation tensor $\mathbf{G}$ requires a transformation law for $\operatorname{Curl}\mathbf{F}^{p}$. Writing $\widehat{\operatorname{Curl}}$ for the curl with respect to $\mathbf{Z}$, the desired transformation law is given by

$$\widehat{\operatorname{Curl}}\,\hat{\mathbf{F}}^{p} = (\det\mathbf{H})\mathbf{H}^{-1}\operatorname{Curl}\mathbf{F}^{p} \tag{12.3}$$

(cf. Cermelli and Gurtin, 2000, Eq. (2.10)).

Consider a change in local reference. Then $\mathbf{G} = (1/J^p)\mathbf{F}^p \,\mathrm{Curl}\,\mathbf{F}^p$ expressed relative to the new reference is $\hat{\mathbf{G}} = (1/\hat{J}^p)\hat{\mathbf{F}}^p \,\hat{\mathrm{Curl}}\,\hat{\mathbf{F}}^p$; thus, by (12.2) and (12.3), *the geometric dislocation tensor is invariant under compatible changes in local reference*: $\hat{\mathbf{G}} = \mathbf{G}$. A similar argument yields the invariance of $\mathbf{G}$ under superposed compatible elastic deformations (Davini, 1986).

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

$$\Phi = \mathscr{F}(\mathbf{F}^p, \nabla\mathbf{F}^p) \tag{12.4}$$

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

$$\mathscr{F}(\hat{\mathbf{F}}^p, \hat{\nabla}\hat{\mathbf{F}}^p) = \mathscr{F}(\mathbf{F}^p, \nabla\mathbf{F}^p). \tag{12.5}$$

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

$$\mathscr{F}(\mathbf{F}^p, \nabla\mathbf{F}^p) = \mathscr{K}(\mathbf{G}). \tag{12.6}$$

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

Sufficiency follows from the invariance of $\mathbf{G}$. To establish necessity, assume that $\mathscr{F}$ is invariant under compatible changes in local reference. Without loss of generality, take $\mathbf{X}_0 = \mathbf{0}$ and restrict attention to local reference changes that map $\mathbf{X} = \mathbf{0}$ to $\mathbf{Z} = \mathbf{0}$. We first show that $\mathscr{F}$ must reduce to a function $\mathscr{F}^*$ of $\mathbf{F}^p$ and $\mathrm{Curl}\,\mathbf{F}^p$:

$$\mathscr{F}(\mathbf{F}^p, \nabla\mathbf{F}^p) = \mathscr{F}^*(\mathbf{F}^p, \mathrm{Curl}\,\mathbf{F}^p). \tag{12.7}$$

Let $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ denote an orthonormal basis. Then $\mathbf{F}^p$ may be written in the form $\mathbf{F}^p = \mathbf{e}_i \otimes \mathbf{f}_i$, with $\mathbf{f}_i = \mathbf{F}^{p\mathrm{T}}\mathbf{e}_i$. (Recall our use of summation convention.) On the space of all smooth vector fields $\mathbf{g}$ there is a one-to-one correspondence between $\mathrm{skw}\,\nabla\mathbf{g}$ and $\mathrm{Curl}\,\mathbf{g}$. Thus, since $\nabla\mathbf{F}^p = \mathbf{e}_i \otimes \nabla\mathbf{f}_i$ and $(\mathrm{Curl}\,\mathbf{F}^p)^{\mathrm{T}} = \mathbf{e}_i \otimes \mathrm{Curl}\,\mathbf{f}_i$ (cf. $(2.8)_5$), to establish (12.7), it suffices to show that

$$\mathscr{F}(\mathbf{F}^p, \mathbf{e}_i \otimes \nabla\mathbf{f}_i) = \mathscr{F}(\mathbf{F}^p, \mathbf{e}_i \otimes \mathrm{skw}\nabla\mathbf{f}_i). \tag{12.8}$$

Let $\mathbf{S}_i = \mathrm{sym}\,\nabla\mathbf{f}_i(\mathbf{0})$ and $(\mathrm{Curl}\,\mathbf{F}^p)^{\mathrm{T}} = \mathbf{e}_i \otimes \mathrm{Curl}\,\mathbf{f}_i$, choose $\mathbf{g}_i$ so that $\mathbf{f}_i \cdot \mathbf{g}_j = \delta_{ij}$, and consider the mapping $\mathbf{X} = \mathbf{Z} - \frac{1}{2}(\mathbf{Z} \cdot \mathbf{S}_k\mathbf{Z})\,\mathbf{g}_k(\mathbf{0})$. Since the gradient $\mathbf{H}(\mathbf{Z}) = \mathbf{1} - \mathbf{g}_k(\mathbf{0}) \otimes (\mathbf{S}_k\mathbf{Z})$ of this mapping satisfies $\mathbf{H}(\mathbf{0}) = \mathbf{1}$, this mapping defines a compatible change in local reference. From (12.2) it follows that under such a change in reference $\hat{\mathbf{f}}_i = \mathbf{H}^{\mathrm{T}}\mathbf{f}_i$. Therefore $\nabla\hat{\mathbf{f}}_i(\mathbf{0}) = \nabla\mathbf{f}_i(\mathbf{0}) + \nabla(\mathbf{H}^{\mathrm{T}}(\mathbf{Z})\mathbf{f}_i(\mathbf{0}))|_{\mathbf{Z}=\mathbf{0}}$, and, because $\mathbf{f}_i \cdot \mathbf{g}_j = \delta_{ij}$, we obtain $\mathbf{H}^{\mathrm{T}}(\mathbf{Z})\mathbf{f}_i(\mathbf{0}) = \mathbf{f}_i(\mathbf{0}) - \mathbf{S}_i\mathbf{Z}$ and $\nabla\hat{\mathbf{f}}_i(\mathbf{0}) = \nabla\mathbf{f}_i(\mathbf{0}) - \mathbf{S}_i = \mathrm{skw}\nabla\mathbf{f}_i(\mathbf{0})$. Thus, since $\hat{\mathbf{F}}^p(\mathbf{0}) = \mathbf{F}^p(\mathbf{0})$, (12.5) implies (12.8). Therefore (12.7) is satisfied.

To establish (12.6), note that, by (12.5) and (12.7), $\mathscr{F}^*(\mathbf{F}^p, \mathrm{Curl}\,\mathbf{F}^p) = \mathscr{F}^*(\hat{\mathbf{F}}^p, \hat{\mathrm{Curl}}\,\hat{\mathbf{F}}^p)$. Consider the *homogeneous* change in reference with gradient $\mathbf{H} \equiv \mathbf{F}^{p-1}(\mathbf{0})$. In this case, $(4.5)_1$, (12.1), and (12.3) yield $\hat{\mathbf{F}}^p(\mathbf{0}) = \mathbf{1}$ and $\hat{\mathrm{Curl}}\,\hat{\mathbf{F}}^p(\mathbf{0}) = \mathbf{G}(\mathbf{0})$, so that $\mathscr{F}^*(\hat{\mathbf{F}}^p, \hat{\mathrm{Curl}}\,\hat{\mathbf{F}}^p) = \mathscr{F}^*(\mathbf{1}, \mathbf{G})$. Thus (12.7) reduces to (12.6).

In view of the remark in the last paragraph of Section 4, a relation $\Phi = \mathscr{F}(\mathbf{F}^e, \mathrm{grad}\,\mathbf{F}^e)$ is invariant under local superposed compatible deformations of the deformed configuration if and only if it has the form $\Phi = \mathscr{K}(\mathbf{G})$.

The Invariance Theorem was arrived at independently by Parry and Šilhavý (1999) and Cermelli and Gurtin (2000). Parry and Šilhavý worked with lattice vectors, but their result is easily translated to one for the field $\mathbf{F}^e$; their work also develops a general theory of elastic invariance involving gradients of order higher than one.

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References

Acharya, A., Bassani, J.L., 2000. Lattice incompatibility and a gradient theory of crystal plasticity. J. Mech. Phys. Solids, 48 (8), 1565–1595.

Asaro, R.J., 1983. Micromechanics of crystals and polycrystals. Adv. Appl. Mech. 23, 1–115.

Bilby, B.A., Bullough, R., Smith, E., 1955. Continuous distributions of dislocations: a new application of the methods of non-Riemannian geometry. Proc. Roy. Soc. London A 231, 263–273.

Cermelli, P., Gurtin, M.E., 2000. On the characterization of geometrically necessary dislocations in finite plasticity. Report 00-CNA-005, Department of Mathematical Sciences, Carnegie Mellon University.

Cermelli, P., Sellers, S., 2000. Multi-phase equilibrium of crystalline solids. J. Mech. Phys. Solids 48/4, 765–796.

Choquet-Bruhat, Y., DeWitt-Morette, C., 1977. Analysis, Manifolds and Physics, vol. 1. North-Holland, Amsterdam.

Davini, C., 1986. A proposal for a continuum theory of defective crystals. Arch. Rational Mech. Anal. 96, 295–317.

Davini, C., Parry, G.P., 1989. On defect preserving deformations in crystals. Int. J. Plasticity 5, 337–369.

Dłużewski, P., 1996. On geometry and continuum thermodynamics of movement of structural defects. Mech. Mater. 22, 23–41.

Eshelby, J.D., 1956. The continuum theory of lattice defects. In: Seitz, F.D., Turnbull, D. (Eds.), Solid State Physics, vol. 3. Academic Press, New York, pp. 79–144.

Fox, N., 1966. A continuum theory of dislocations for single crystals. J. Inst. Math. Appl. 2, 285–298.

Gurtin, M., 1972. The linear theory of elasticity. In: Truesdell, C. (Ed.), Mechanics of Solids II, Handbuch der Physik 6/a2. Springer, Berlin.

Kalinindi, S.R., Anand, L., 1993. Large deformation simple compression of a copper single crystal. Metall. Trans. 24A, 989–992.

Kocks, U.F., Tomé, C.N., Wenk, H.-R., 1998. Texture and Anisotropy. Cambridge University Press, Cambridge.

Kondo, K., 1952. On the geometrical and physical foundations of the theory of yielding. Proceedings Japan National Congress of Applied Mechanics, vol. 2, pp. 41–47.

Kondo, K., 1955. Non-Riemannian geometry of imperfect crystals from a macroscopic viewpoint. In: Kondo, K. (Ed.), RAAG Memoirs of the Unifying Study of Basic Problems in Engineering and Physical Science by Means of Geometry, vol. 1. Gakuyusty Bunken Fukin-Kay, Tokyo.

Kröner, E., 1960. Allgemeine Kontinuumstheorie der Versetzungen und Eigenspannungen. Arch. Rational Mech. Anal. 4, 273–334.

Kuhlmann-Wilsdorf, D., 1989. Theory of plastic deformation: properties of low energy dislocation structures. Mater. Sci. Eng. 113A, 1–41.

Lee, E.H., 1969. Elastic-plastic deformation at finite strains. J. Appl. Mech. 36, 1–6.

Naghdi, P.M., Srinivasa, A.R., 1993. A dynamical theory of structured solids. I Basic developments. Philos. Trans. Roy. Soc. London A 345, 425–458.

Noll, W., 1967. Materially uniform simple bodies with inhomogeneities. Arch. Rational Mech. Anal. 27, 1–32.

Nye, J.F., 1953. Some geometrical relations in dislocated solids. Acta Metall. 1, 153–162.

Parry, G.P., Šilhavý , M., 1999. Elastic scalar invariants in the theory of defective crystals. Proc. Roy. Soc. London A 455, 4333–4346.

Prantil, V.C., Jenkins, J.T., Dawson, P.R., 1993. An analysis of texture and plastic spin for planar polycrystals. J. Mech. Phys. Solids 41, 1357–1382.

Schwartz, A.J., Stölken, J.S., King, W.E., Campbell, W.E., Lassila, D.H., Sun, S., Adams, B.L., 1999. Analysis of compression behavior of a [011] Ta single crystal with orientation imaging microscopy and crystal plasticity. Report UCRL-JC-133402, Lawrence Livermore National Laboratory.

Sun, S., Adams, B.L., King, W.E., 2000. Observations of lattice curvature near the interface of a deformed aluminum bicrystal. Philos. Mag. A 80, 9–25.

Sun, S., Adams, B.L., Shet, C., Saigal, S., King, W., 1998. Mesoscale investigation of the deformation field of an aluminum bicrystal. Scripta Mater. 39, 501–508.

Synge, J.L., 1960. Classical dynamics. In: Flügge, S. (Ed.), Principles of Classical Mechanics and Field Theory, Handbuch der Physik 3/1. Springer, Berlin.

Teodosiu, C., 1970. A dynamical theory of dislocations and its applications to the theory of the elastic-plastic continuum. In: Simmons, J.A. et al. (Eds.), Proceedings of Conference on Fundamental Aspects of Dislocation Theory, Washington 1969, N.B.S. Spec. Publ. 317/2, 837–876.

Teodosiu, C., 1982. Elastic Models of Crystal Defects. Springer, Berlin.