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Lattice incompatibility and a gradient theory of crystal plasticity

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Abstract

In the finite-deformation, continuum theory of crystal plasticity, the lattice is assumed to distort only elastically, while generally the elastic deformation itself is not compatible with a single-valued displacement field. Lattice incompatibility is shown to be characterized by a certain skew-symmetry property of the gradient of the elastic deformation field, and this measure can play a natural role in a nonlocal, gradient-type theory of crystal plasticity. A simple constitutive proposal is discussed where incompatibility only enters the instantaneous hardening relations, and thus the incremental moduli, which preserves the classical structure of the incremental boundary value problem.

1. Introduction

Motivated by various observations of scale effects involving plastic deformation (examples given below), this paper seeks to quantitatively interpret and account for the manifestations of an imperfect lattice structure within the context of the conventional continuum theory of crystal plasticity (Rice, 1971; Hill and Havner, 1982; Asaro, 1983; Havner, 1992; Bassani, 1994). It is well known that the movement of dislocations causes plastic flow, while the presence of lattice defects

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impedes such flow and leads to work hardening; an example of the latter is the forest hardening mechanism arising from the dislocations themselves. In the continuum theory of crystal plasticity, the presence and motion of dislocations are not explicitly recognized, their effects being modeled by the crystallographic slips which define, along with the lattice vectors, the evolution of plastic deformation of the crystal. Quite commonly, these slip variables are also assumed to control the evolution of material hardening.

As will be shown in this paper, the elastic distortion of the lattice is not, in general, compatible with a deformation, i.e. one that is derivable from a continuously differentiable displacement field, while it is capable of representing certain lattice imperfections, e.g. those associated with geometrically-necessary dislocations (Nye, 1953), via an analysis of the incompatibility of this deformation. We work with the hypothesis that this incompatibility is not accounted for in the conventional theory, inasmuch as the effects of such imperfections on hardening are ignored when one assumes that hardening only depends on the crystallographic slip variables whose evolution is unimpeded by incompatible lattice deformations. The lattice incompatibility associated with these defects is characterized essentially by the gradient of the (inverse of the) elastic distortion field (Bilby et al., 1955), and when incorporated in the hardening response it introduces a material length-scale in the theory simply on dimensional grounds. In this paper, we establish the necessary and sufficient measure of lattice incompatibility from both a simple calculus argument and an argument in the setting of a non-Riemannian geometry.

Several distinct examples of observed scale effects follow (see, Fleck and Hutchinson, 1997). The first arises in so-called nano-indentation measurements where the inferred hardness increases as the indentation decreases in size from roughly below tens of microns to fractions of a micron (see Stelmashenko et al., 1993; Ma and Clarke, 1995). Another is the increase in overall hardness of metals containing hard particles, as the size of those particles decreases in the sub-micron range while the overall volume fraction is held fixed (see Ebeling and Ashby, 1966; Brown and Ham, 1971). Recently, Cleveringa et al. (1997) have predicted the latter behavior using a dislocation dynamics simulation. A third example is the patterning of coarse-slip microstructures, particularly the thickness and spacing of the slip bands (see Piercy et al., 1955; Basinski and Basinski, 1979; Chang and Asaro, 1981; Bassani, 1994). Also related are persistent slip band microstructures (see, e.g., Glazov and Laird, 1995). All of these scale effects are found even for high-purity single crystals. In polycrystals, the Hall–Petch effect is widely observed: at a given overall strain the overall stresses tend to increase as the grain size decreases (Hall, 1951; Petch, 1953; Dai and Parks, 1997). Finally, we also cite the observation that the thermally-induced stresses in thin films on a stiff substrate tend to increase with decreasing film thickness (see Nix, 1989).

The work presented here was motivated by a desire to establish a connection between the theory of continuous distributions of defects and internal stress (Kondo, 1955, 1958, 1962, 1968; Nye, 1953; Bilby et al., 1955; Kröner and Seeger, 1959), the theory of materially uniform inhomogeneous elastic bodies (Truesdell and Noll, 1965), the notion of defect-preserving deformations in crystals (Davini and Parry, 1989), and the continuum theory of crystal plasticity. While the literature on continuous distributions of defects (and compatibility for that matter) relies primarily on tools from differential geometry, we obtain the essential results in this paper merely from the use of tools from linear algebra and calculus. We show that the physical implications of the underlying kinematics of crystals provides a constitutive length scale from within, but undetermined by, the theory itself as Fleck et al. (1994) observed in the setting of infinitesimal kinematics.

With the total deformation gradient multiplicatively decomposed into elastic and plastic parts, i.e. $\mathbf{F} = \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{p}}$ (see, e.g., Lee and Liu, 1967; Willis, 1969; Rice, 1971), we analyze the incompatibility associated with the mapping of the reference lattice under the field $\mathbf{F}^{\mathrm{e}}$. Since the lattice vectors in the undeformed reference may be considered as material vectors under such a mapping, the image of these vectors is taken to represent the deformed lattice. Alternatively, we analyze the relationship between the incompatibility of the field $\mathbf{F}^{\mathrm{e}-1}$ on the current configuration and the closure failure associated with the mapping of a closed material curve of the current configuration onto an intermediate configuration. Tensorial measures of incompatibility, that are motivated physically in terms of the distorted lattice (which is not easily visualized because of the inherent nature of incompatibility), are defined from elements of calculus and differential geometry. One such measure involves a certain skew-symmetric gradient of $\mathbf{F}^{\mathrm{e}-1}$ on the current configuration.

On associating the incompatibility of $\mathbf{F}^{\mathrm{e}}$ or $\mathbf{F}^{\mathrm{e}-1}$ with the presence of defects in solids, we then propose to incorporate a measure of the incompatibility into the instantaneous hardening response which can enter either a rate-independent or rate-dependent flow rule. In the case of rate-independent behavior, introducing a measure of incompatibility only in the so-called tangent (incremental) moduli leaves the nominal stress-rate response in the material as a homogeneous function of degree one in the deformation gradient rate. As a result, the structure of the boundary value problem (bvp) of the conventional theory and all associated results on uniqueness of the problem of rate-equilibrium for the rate-independent material (Hill, 1958, 1959, 1978) are retained. This is in contrast to the Fleck and Hutchinson (1993, 1997) theory, which involves higher-order stresses, and other gradient theories (e.g., Aifantis, 1987). The abovementioned simplicity in the structure of the bvp of incremental equilibrium due to the addition of non-locality only in the incremental moduli, and its thermodynamic justification, in the case of a second-deformation-gradient dependence of material response, was pointed out in an earlier work by Acharya and Shawki (1995).

We also argue on thermodynamical grounds that the incompatibility measures cannot explicitly enter into the constitutive equations for the stress when the body is assumed to be incapable of performing work due to higher-order stresses, thus justifying our inclusion of the incompatibility tensor in the hardening response, and hence, the incremental moduli. Furthermore, with this non-locality in material response an intrinsic length scale is naturally introduced into the constitutive relations. The paper closes with the derivation of the frame-indifferent measures of the identified incompatibilities.

2. Earlier work

In this section we briefly summarize *our* interpretation of some aspects of the earlier work of Kondo, Nye, Bilby, Kröner, Noll and Davini and Parry, particularly those aspects that relate to the point of view of this paper. Nevertheless, the remainder of the paper is self contained and does not rely on this interpretation, although in order to gain full perspective this section is highly recommended to the reader. This section is not meant to be a comprehensive literature survey of all work based on the theory of continuous distributions of dislocations; it is a review of those seminal works in the literature that have had the most profound impact on our thinking on this subject.

The theory of continuous distributions of defects begins with the work of Kondo (1955, 1958, 1962, 1968, 1963) and earlier references therein, who assumes a metrically incompatible deformation (i.e., a positive-definite symmetric second-order tensor field on the body which cannot be expressed as the right Cauchy–Green strain tensor of a deformation) to be the mathematical representation of the onset of inelasticity in a material. He interprets yielding as the first onset of a non-vanishing Euler–Schouten curvature tensor on the material manifold; a tensor which is closer to the intuitive notion of curvature of a manifold, as viewed from an enveloping space, than the intrinsic Riemann–Christoffel curvature of the metric which does not distinguish between isometric deformations of the manifold. In this approach, Kondo *associates a Riemannian geometry, i.e., a geometry with a torsionless connection, with inelasticity in the material*. However, in the vast body of work produced by Kondo and his co-workers, the use of Riemannian, non-Riemannian and Finslerian geometric approaches to the analysis of inelasticity is proposed.

Nye (1953) analyzes the problem of determining the arrangement of dislocations in a crystal containing an arbitrary distribution of dislocation lines, such that the average of the stresses over distances that are large compared to the mean dislocation spacing is zero. Nye assumes that *the lattice is unstrained but that the local rotation field that the lattice vectors are subjected to varies with position*. *A tensor of dislocation density* is introduced which gives, when integrated over any surface of the body, the Burgers vector of all the dislocation lines threading that surface.

A more general analysis of the idea of Nye is given by Bilby et al. (1955), where a crystal with a continuous distribution of dislocations is visualized as a body equipped with three director vectors at each point, called lattice vectors. A general vector field on the reference lattice is defined to be 'parallel' if the components of the field at each point, w.r.t. the lattice triad at the corresponding points, are identical. Clearly, if the lattice triad at each point of the reference is not the same, then the abovementioned 'parallel' field of vectors is not parallel in the ordinary Euclidean sense. With this definition of parallelism in the reference lattice at hand, the images of parallel reference lattice vectors under the lattice deformation are said to be parallel in the deformed lattice configuration. The analysis of the spatial gradient of a field of parallel vectors in the deformed lattice configuration along a curve in the material manifold yields a linear connection whose torsion is identified with the dislocation density. In Bilby's work, *the dislocation density tensor is generated from an analysis of the closure failure associated with the 'parallel', reference lattice image of a closed curve in the deformed lattice*. Due to the assumed smoothness and invertibility of the lattice deformation field, the affine curvature tensor of the linear connection vanishes. The foregoing fact is crucial in generating the relationship between the lattice strain incompatibility tensor and the dislocation density, which is a fundamental relationship in solving the problem of residual stresses. Bilby (1960) makes a clear distinction between a compatible material deformation generated from a displacement field and incompatible lattice or dislocation deformations specified by symmetric second-order tensor valued strain fields, in the context of small deformations.

The main contribution of Kröner and Seeger (1959) and earlier references therein to the theory of continuous distributions of dislocations *is in the analysis of internal stresses due to dislocation distributions in the material*. For small strains and an infinite body (Kröner, 1981), the dislocation density is assumed to be known. The equation of equilibrium and a differential equation relating the elastic strain incompatibility field to the dislocation density are solved to generate the state of internal stress in the medium. For the problem of non-linear elasticity, Kröner and Seeger derive a relationship between the Eulerian strain tensor and the defining connection representing the presence of dislocations. This relationship, along with the equation of equilibrium, forms the governing equations for determining the internal stresses. Eshelby (1956) indicates a solution procedure, in the case of infinitesimal deformations, for dealing with bodies of finite extent.

Truesdell and Noll (1965) define a *materially uniform* body as one whose density and stress-response functional are uniform over the body, but where such a uniform response may not be achievable from a coherent global configuration (i.e., a configuration in one piece) of the body. To achieve the uniformity of response, the body would typically need to be cut into small parts. If, however, such uniformity in the stress response is achievable from a coherent configuration, then such a body is called homogeneous and the configuration is called a homogeneous reference. Noll's work is closely related to the notion of a multiplicative decomposition of the deformation gradient ($\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$) with a uniform stress-response function associated with the intermediate configuration of finite elastoplasticity. In fact, this association, with a direct reference to Noll's theory, was pointed out independently by Fox (1968), who also derived an expression for the dislocation density in terms of the second-order tensor field defining the material uniformity. In the setting of our work, a crystal can be brought to a state with uniform stress-response by cutting it into small pieces (to let the lattice relax to its original condition in each of these pieces) and rigidly rotating each piece so that the lattice orientation is identical in the pieces. The *collection of all these pieces is the intermediate configuration of the continuum theory of crystal plasticity and, alternatively, a materially uniform reference in the sense of Noll.*

We also note here that with the exception of the work of Fox (1968), all of the abovementioned works are primarily concerned with the representation of a 'static' theory of dislocation distributions in the body.

Davini and Parry (1989, 1991) and Parry (1992) pose the question of the kinematical relationship between two configurations of a crystal which are not related by an elastic deformation but have the same defectiveness. They define the notion of defectiveness by a complete list of kinematical objects which remain invariant under elastic deformations of the crystal. The 'completeness' of the set refers to the fact that all other such invariants can be expressed in terms of the elements of the set. They find that their question has non-null content in that the answer comprises deformations (called 'neutral' by them) which are not elastic but keep the defectiveness invariant. These neutral deformations characterize the process of slip rearrangements in real crystal lattices. For processes of slip in perfect crystals (states with no defectiveness), they also derive the conventional 'multiplicative decomposition' of the deformation gradient of finite elastoplasticity.

While Davini and Parry concern themselves mostly with the question of characterizing deformations that keep the 'defectiveness' constant, the lattice incompatibility measures to be proposed in our paper characterize some kinematical aspects of plastic deformation of crystals in which the defectiveness, in their terminology, changes; however, measures closely related to the one proposed in this paper arise in their work in connection with the characterization of kinematic measures that remain unaltered due to elastic deformation.

3. Notation and terminology

As far as possible we try to use coordinate and component free notation. Vectors are represented by boldface, lowercase Latin letters; tensors, by boldface, uppercase Latin letters. Real numbers (both physical scalars and components of tensors) are denoted by italicized symbols as are tensor components with appropriate subscripts and superscripts. For the most part, Latin indices denote Cartesian components of tensors (as used extensively throughout in Section 5.1), while Greek indices denote components of tensors with respect to general base vectors (as used extensively throughout Section 5.2).

Scalar inner products are denoted by a single dot between vectors. Time derivatives of a quantity are represented by a dot above a quantity or a superscript dot after a bracket enclosing the quantity. Summation over repeated tensor indices is implied.

The primary definition of a third-order tensor is taken to be that of a linear transformation on the space of three-dimensional vectors to the space of second-order tensors on the foregoing vector space. A tensor (second-order, third-order) placed adjacent and to the left of a vector denotes the result of the tensor acting on the vector. The tensor product of three vectors $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$, denoted by $\mathbf{u} \otimes \mathbf{v} \otimes \mathbf{w}$, is a third-order tensor defined by the rule,

$$(\mathbf{u} \otimes \mathbf{v} \otimes \mathbf{w})\mathbf{a} = (\mathbf{a} \cdot \mathbf{w})\mathbf{u} \otimes \mathbf{v},$$

for all vectors $\mathbf{a}$. For three bases $\{\mathbf{e}_\alpha\}$, $\{\mathbf{g}_\beta\}$, $\{\mathbf{f}_\gamma\}$, with corresponding dual bases $\{\mathbf{e}^\alpha\}$, $\{\mathbf{g}^\beta\}$, $\{\mathbf{f}^\gamma\}$, a third-order tensor $\mathbf{B}$ has the representation,

$$\mathbf{B} = B^{\alpha\beta\gamma}\mathbf{e}_\alpha \otimes \mathbf{g}_\beta \otimes \mathbf{f}_\gamma,$$

where $B^{\alpha\beta\gamma} = \mathbf{e}^\alpha \cdot (\mathbf{B}\mathbf{f}^\gamma)\mathbf{g}^\beta$. For a second-order tensor $\mathbf{A}$ and a third-order tensor $\mathbf{B}$, the product $\mathbf{AB}$ is a third-order tensor defined as

$$(\mathbf{AB})\mathbf{v} = \mathbf{A}(\mathbf{Bv}) \quad \text{for all vectors } \mathbf{v}.$$

In stating our mathematical results on the construction of functions over some domain, by a ‘global’ result we mean its validity over the entire domain. By a ‘local’ result we mean the validity of the result in some open set around a point of the domain. Often, the local results hold for every point of the domain.

4. Elements of crystal kinematics

We adopt the standard definition for a continuum configuration of a body of a single crystal to mean a *collection of material points and slip vectors*, i.e. pairs of vectors representing a slip direction and a slip plane normal for each slip system defined at every point. For the sake of simplicity, the reference configuration R is taken to be the stress-free body of perfect crystal and, therefore, the slip vectors do not vary from point to point in R. Any other configuration C of the body is defined by (i) a smooth, locally invertible deformation of material points in R to material points in C (with deformation gradient denoted generically by $\mathbf{F}$) and (ii) a sufficiently smooth, invertible, second-order tensor-valued *elastic deformation field* ($\mathbf{F}^{\mathrm{e}}$) which relates lattice vectors, e.g. the slip vectors, in R to their counterparts in C at every point of R.

Let $\mathbf{X}$ represent the generic point in the reference configuration and $\mathbf{x}$ its counterpart in C; also let $\mathbf{n}_0^\kappa$ and $\mathbf{n}^\kappa$ be the normals to the slip plane at $\mathbf{X}$ and $\mathbf{x}$ and $\boldsymbol{m}_0^\kappa$ and $\mathbf{m}^\kappa$ the slip directions at $\mathbf{X}$ and $\mathbf{x}$, respectively, for slip system κ. Then (Rice, 1971; Hill and Havner, 1982; Havner, 1992; Bassani, 1994):

$$\mathbf{x} = \mathbf{x}(\mathbf{X}), \quad \mathrm{d}\mathbf{x} = \mathbf{F}\,\mathrm{d}\mathbf{X} \tag{1a}$$

$$\mathbf{m}^\kappa = \mathbf{F}^{\mathrm{e}}\mathbf{m}_0^\kappa \tag{1b}$$

$$\mathbf{n}^\kappa = \mathbf{F}^{\mathrm{e}-T}\mathbf{n}_0^\kappa \tag{1c}$$

where the deformation gradient $\mathbf{F}$ has been decomposed into elastic and plastic parts. Alternative forms for the evolution of slip vectors have also been adopted, e.g. keeping them unit vectors, but in all cases they evolve only with part of the deformation (see Asaro and Rice, 1977; Havner, 1992). The multiplicative decomposition is commonly adopted: $\mathbf{F} = \mathbf{F}^{e}\mathbf{F}^{p}$ along with the prescription for the plastic part of the velocity gradient:

$$\mathbf{L}^{p} = \mathbf{F}^{e}\dot{\mathbf{F}}^{p}\mathbf{F}^{p-1}\mathbf{F}^{e-1} = \sum_{\kappa}\dot{\gamma}^{\kappa}\mathbf{m}^{\kappa}\otimes\mathbf{n}^{\kappa} \tag{2}$$

where $\dot{\gamma}^{\alpha}$ denotes the slip rate on system α.

The configuration C is an elastic configuration if $\mathbf{F}^{e} = \mathbf{F}$ over the whole of R; otherwise it is thought of as elastic-plastic. If the field $\mathbf{F}^{e-1}$ on C or $\mathbf{F}^{e}$ on R is non-integrable in the sense that no deformation of C or R, respectively, can have a deformation gradient that matches these second-order tensor fields, then the *intermediate configuration* is incompatible and the geometry induced on the crystal by the intermediate configuration (the incompatibly distorted lattice) is non-Riemannian in the sense that suitably defined linear connections based on the mappings $\mathbf{F}^{e-1}$ on C or $\mathbf{F}^{e}$ on R are asymmetric (e.g., Bilby et al., 1955). Consistent with Eqs. (1b) and (1c), we emphasize that the lattice distortion is purely elastic, which is to say that the reference and intermediate lattice configurations are identical. Inasmuch as the intermediate configuration can be defined by the field $\mathbf{F}^{e-1}$ on C for both material and lattice or, equivalently, by 'material distortion' $\mathbf{F}^{p}$ on R with the identity mapping for lattice vectors, there is no unique meaning that can be assigned to it due to the lack of a smooth mapping of points. Consequently, one cannot easily visualize the intermediate configuration since it is, in general, broken up. Of course, if $\mathbf{F}^{e}$ is uniform (constant) then a compatible lattice deformation and intermediate configuration always exist.

As noted above, in general the fields $\mathbf{F}^{e-1}$ on C and $\mathbf{F}^{p}$ on R do not correspond to a smooth, one-to-one mapping of points. In the next section we proceed to establish the circumstances under which they do, i.e. when a second-order tensor field is the gradient of a vector field. Two proofs on the compatibility of an invertible second-order tensor field with a deformation of points are presented in the next section. The first proof is based upon a standard result of calculus. The second is primarily geometrical in nature and it provides an equivalent condition for local compatibility, i.e. compatibility in a neighborhood of a point of the domain of definition of the tensor field. This proof requires stronger smoothness hypotheses on the tensor field than the first proof, which is analytical and provides conditions of equivalence for global compatibility (and consequently local compatibility). From either point of view, a natural measure(s) of incompatibility emerges in terms of a certain gradient of $\mathbf{F}^{e-1}$ on C (or of a gradient of $\mathbf{F}^{e}$ on R).

We present the second proof both to provide insight into some of the more subtle aspects of incompatibility and partly due to the differential-geometric tradition of the subject. The combination of the simple viewpoint of deformation-gradient compatibility and the interrelations between two dominant streams of thought (Bilby et al., 1955; Truesdell and Noll, 1965) on the subject has certainly sharpened our understanding of the issues involved.

In the next section we also define the presence of defects in the body, as understood in the theory of continuous distributions of dislocations, and relate the incompatibility measures to the presence of geometrically-necessary dislocations. This result provides tensorial measures, defined in terms of the gradient of the field $\mathbf{F}^{e-1}$ or $\mathbf{F}^{e} = \mathbf{F}\mathbf{F}^{p-1}$ on the relevant configurations, that characterize the presence of these defects. Furthermore, if the constitutive response is taken to depend on incompatibility via such a gradient measure, then a length scale must enter the material response on dimensional grounds. Finally, we note that although $\mathbf{L}^{p}$ given in Eq. (2) is expressed as a linear combination involving the slip rates on all systems, neither $\mathbf{F}^{p}$ nor $\mathbf{F}^{p-1}$ can be written as a sum involving the total slips. This fact becomes important if one tries to associate a portion of incompatibility with individual slip systems which will also be addressed below.

5. Mathematical characterization of incompatibility

The basic question posed is the natural one related to compatibility: *Given a sufficiently smooth invertible second-order tensor field* $\mathbf{A}(\mathbf{x})$ *on an arbitrary reference* K *with points denoted* $\mathbf{x}$*, what are the conditions that have to be satisfied, such that there exists a position vector field* $\boldsymbol{y}$ whose deformation gradient field, $\partial\mathbf{y}/\partial\mathbf{x}$, matches $\mathbf{A}$?

The first approach to answering this question, which is followed in Section 5.1, is based on elementary analysis and establishes the requirements for *global* compatibility. We then present another point of view in Section 5.2 that begins with a statement of mapping a natural basis of an arbitrary coordinate system for K, and goes on to study the differential geometry of the space spanned by the mapped vectors. In particular, $\mathbf{A}$ maps the lattice-vector fields on K to another 'space' whose compatibility with K is to be probed. This approach, as far as we can establish, leads only to a statement of local compatibility. From the analysis of compatibility, one is immediately led to equivalent measures of incompatibility: Nye's dislocation density tensor, Cartan's torsion tensor, and a certain skew-symmetric gradient of $\mathbf{A}$.

5.1. The calculus argument

In this section we derive conditions for *global* compatibility of a continuously differentiable invertible second-order tensor field $\mathbf{A}$ on K, where K is assumed to be simply connected. (A similar argument, in terms of 'lattice correspondence functions' and in a different degree of detail, is presented in Bilby, 1960.) For convenience, we choose a rectangular Cartesian coordinate system for K with basis $\{\mathbf{e}_i\}$, and express the components of $\mathbf{A}$ with respect to it as

$$A_{\cdot j}^{i} = \mathbf{e}^{i} \cdot \mathbf{A}\mathbf{e}_{j}, \tag{3}$$

where the distinction in the position of indices is unnecessary, but we retain it to maintain consistency with general tensor notation. As the notation suggests, if it is possible to regard the basis vectors $\{\mathbf{e}_i\}$ as the lattice vectors, then $A_{\cdot j}^{i}$ is the i^{th} Cartesian component of the j^{th} deformed lattice vector.

To begin, we suppose that there exists a continuously differentiable deformation of K, denoted by $\mathbf{y}$, whose deformation gradient matches $\mathbf{A}$, i.e. $\partial\mathbf{y}/\partial\mathbf{x} = \mathbf{A}$ on K. Since $\mathbf{A}$ is taken to be continuously differentiable, $\mathbf{y}$ is twice continuously differentiable. Now, let the representation of $\mathbf{y}$ as a field of position vectors with respect to the chosen coordinate system and arbitrarily chosen origin be

$$\mathbf{y} = y^l \mathbf{e}_l.$$

Then the functions y^k are twice continuously differentiable with respect to the coordinates and

$$A_{\cdot j,\,k}^{i} = \left(\mathbf{e}^i \cdot \mathbf{A}\mathbf{e}_j\right)_{,k} = \left(\mathbf{e}^i \cdot \frac{\partial \mathbf{y}}{\partial \mathbf{x}}\mathbf{e}_j\right)_{,k} = \left(\mathbf{e}^i \cdot \mathbf{y}_{,j}\right)_{,k} = y^i_{,jk} = y^i_{,kj} = A^i_{\cdot k,\,j}. \tag{4}$$

Conversely, assume that $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$ on K. Consider the function y^i on K given by the line integral

$$y^i\left(x^1, x^2, x^3\right) = \int_{\left(x_0^1,\, x_0^2,\, x_0^3\right)}^{\left(x^1,\, x^2,\, x^3\right)} A_{\cdot j}^{i}\, \mathrm{d}x'^{\,j}, \tag{5a}$$

where $\mathbf{x}_0 = x_0^i \mathbf{e}_i$ is an arbitrarily chosen fixed point of K and $\mathbf{x} = x^i \mathbf{e}_i$ is any other point of K. Also, the line integral is evaluated on any arbitrarily chosen piecewise smooth curve. Now, since $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$ on K by hypothesis, an application of the classical Stokes theorem for simply connected domains proves that the line integral above is path independent, and then it can be shown from the definition of y^i that

$$y^i_{,j} = A_{\cdot j}^{i}. \tag{5b}$$

Defining a deformation $\mathbf{y}$ of K (as a field of position vectors) from the y^i just constructed according to Eq. (5) with $\mathbf{y} = y^l \mathbf{e}_l$, we find that $\mathbf{A} = \partial\mathbf{y}/\partial\mathbf{x}$ since both have the same components with respect to the basis $\{\mathbf{e}_l\}$.

Hence, we have established that if $\mathbf{A}$ is continuously differentiable on K and if K is simply connected, then $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$ and global (and hence, local) compatibility of $\mathbf{A}$ are equivalent assertions. Therefore, in terms of Cartesian components a natural measure of incompatibility of $\mathbf{A}$ is

$$\alpha^{ip} = \mathrm{e}^{pjk} A_{\cdot k,\,j}^{i}, \tag{6}$$

where e^{pjk} is the alternating symbol and $\mathbf{A}$ is compatible iff $\alpha^{ip} = 0$. In the next section we will show that symmetry of the 'connection' associated with $\mathbf{A}$ also follows if $\mathbf{A}$ is compatible.

In closing this section we return to the setting (and notation) of crystal plasticity as defined above and establish the relationship with Nye's geometrically necessary dislocations and the measure of their density. Incompatibility in the lattice deformation, $\mathbf{F}^{\mathrm{e}}$ (see Eqs. (1b) and (1c)), can be associated with defects in the solid, in particular with the so-called geometrically necessary dislocations (Nye, 1953) which, for example, can lead to polygonization (Nabarro, 1967; Gilman, 1955) or account for the presence of grain boundaries (Kröner, 1981). There is a relation between the incompatibility defined by $\mathbf{F}^{\mathrm{e}-1}$ on C and the presence of geometrically-necessary dislocations in the solid which is motivated by the fact that if there exists a surface element in C that is threaded by an excess of dislocation lines of one sign, then it is not possible to compatibly map such a surface element in C to a region with a perfect lattice structure. Motivated by the theory of continuous distribution of dislocations, we define the *cumulative Burgers vector* of all dislocation lines that belong to the interior of a loop formed by a closed curve C by

$$\mathbf{b} = \oint_C \mathbf{F}^{\mathrm{e}-1}\,\mathrm{d}\mathbf{x}, \tag{7a}$$

or using Stokes' theorem (and in rectangular Cartesian component form)

$$b_i = \oint_C F^{\mathrm{e}-1}_{ij}\,\mathrm{d}x_j = \int_S \mathrm{e}^{pjk} F^{\mathrm{e}-1}_{ik,\,j} r_p\,\mathrm{d}S, \tag{7b}$$

where $\mathbf{r}$ is the unit normal to a surface S whose boundary is the curve C. With $\mathbf{A}$ in Eq. (6) associated with $\mathbf{F}^{\mathrm{e}-1}$, the resulting $\boldsymbol{\alpha}$ is Nye's dislocation density tensor and $\mathbf{b} = \int_S \boldsymbol{\alpha r}\,\mathrm{d}S$. A non-vanishing Burgers vector at a point of C can be interpreted as the closure failure associated with the image, in the 'intermediate configuration', of a closed curve in C that bounds an infinitesimal element of area containing that point. Hence, we define the presence of geometrically necessary dislocations in C by the existence of at least one closed curve in C for which the cumulative Burgers vector is non-vanishing. With this definition in hand, the equivalence of the compatibility of $\mathbf{F}^{\mathrm{e}-1}$ on C with vanishing cumulative Burgers vector for all closed curves in C is easily established along with the obvious relationship between the incompatibility of $\mathbf{F}^{\mathrm{e}-1}$ and the presence of geometrically necessary dislocations.

5.2. The lattice-geometric argument

The technical content of this section follows closely that of Truesdell and Noll (1965, Section 34, p. 88). However, we believe that the conceptual standpoint gains significantly in simplicity when the problem is posed as one of compatibility of a prescribed 'deformation gradient' field, in comparison to their query on the homogeneity of the somewhat abstract 'materially uniform reference.' Some useful results on non-Riemannian geometry can be found in Eisenhart (1927), Synge and Schild (1949), and Laugwitz (1965). In order to fully reveal the nature of the geometry under consideration, it is useful to work in a general coordinate system, and with this purpose in mind, base vectors and components of tensors will be denoted with Greek indices.

Let $\{x^\alpha\}$ be a general coordinate system for three-dimensional ambient space, which is understood to be the parametrizing coordinate system for K, and let $\{\mathbf{c}_\alpha\}$ denote its natural basis, i.e., $\mathbf{c}_\alpha = \partial\mathbf{x}/\partial x^\alpha$, which can be the lattice vectors in the perfect crystal R. Define the mapped basis vectors

$$\mathbf{d}_\alpha = \mathbf{A}\mathbf{c}_\alpha. \tag{8}$$

Since $\mathbf{A}$ is invertible, $\mathbf{d}_\alpha$ is a basis and $\mathbf{d}_{\alpha,\,\beta}$, where the comma denotes the partial derivative with respect to coordinates (x^β), can be expressed as

$$\mathbf{d}_{\alpha,\,\beta} = \Gamma^\gamma_{\alpha\beta}\mathbf{d}_\gamma. \tag{9}$$

With $\{\mathbf{d}^\gamma\}$ denoting the dual basis of $\{\mathbf{d}_\gamma\}$,

$$\Gamma^\gamma_{\alpha\beta} = \mathbf{d}^\gamma \cdot \mathbf{d}_{\alpha,\,\beta}. \tag{10}$$

In order to determine the geometric significance of the array $\Gamma^\gamma_{\alpha\beta}$, we consider a change of coordinates on K and examine its transformation rule. Let the new coordinate system be denoted by $\{\bar{x}^\alpha\}$. Then

$$\bar{\mathbf{c}}_\alpha = \frac{\partial x^\mu}{\partial \bar{x}^\alpha}\mathbf{c}_\mu \quad \text{and} \quad \bar{\mathbf{d}}_\alpha = \mathbf{A}\bar{\mathbf{c}}_\alpha = \mathbf{A}\left(\frac{\partial x^\mu}{\partial \bar{x}^\alpha}\mathbf{c}_\mu\right) = \frac{\partial x^\mu}{\partial \bar{x}^\alpha}\mathbf{d}_\mu.$$

Consequently, differentiating the last relation with repect to $\bar{x}^\beta$

$$\begin{aligned}\bar{\mathbf{d}}_{\alpha,\,\beta} &= \frac{\partial^2 x^\mu}{\partial \bar{x}^\alpha \partial \bar{x}^\beta}\mathbf{d}_\mu + \frac{\partial x^\mu}{\partial \bar{x}^\alpha}\frac{\partial x^\omega}{\partial \bar{x}^\beta}\Gamma^\gamma_{\mu\omega}\mathbf{d}_\gamma = \left[\frac{\partial^2 x^\gamma}{\partial \bar{x}^\alpha \partial \bar{x}^\beta} + \frac{\partial x^\mu}{\partial \bar{x}^\alpha}\frac{\partial x^\omega}{\partial \bar{x}^\beta}\Gamma^\gamma_{\mu\omega}\right]\frac{\partial \bar{x}^\rho}{\partial x^\gamma}\bar{\mathbf{d}}_\rho \\ &\equiv \bar{\Gamma}^\rho_{\alpha\beta}\bar{\mathbf{d}}_\rho\end{aligned}$$

where Eq. (9) has been used. Since $\bar{\mathbf{d}}_\rho$ is a basis we find that the array $\Gamma^\gamma_{\alpha\beta}$ satisfies the transformation rule (with respect to the coordinate systems $\{x^\alpha\}$ and $\{\bar{x}^\alpha\}$) for a *linear connection* given by

$$\bar{\Gamma}^\rho_{\alpha\beta} = \left[\frac{\partial^2 x^\gamma}{\partial \bar{x}^\alpha \partial \bar{x}^\beta} + \frac{\partial x^\mu}{\partial \bar{x}^\alpha}\frac{\partial x^\omega}{\partial \bar{x}^\beta}\Gamma^\gamma_{\mu\omega}\right]\frac{\partial \bar{x}^\rho}{\partial x^\gamma}. \tag{11}$$

Of course, if x^α and $\bar{x}^\beta$ are both Cartesian coordinate systems, then the term involving the second derivative in Eq. (11) is identically zero, indicating that the connection transforms tensorially *only* with respect to Cartesian coordinate systems.

Now, if there exists a continuously differentiable deformation $\mathbf{y}$ of K such that

$$\mathbf{A} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \tag{12}$$

in K (which implies $\mathbf{A}$ is compatible), then $\mathbf{y}$ is twice continuously differentiable. With Eq. (12) and $\mathbf{c}_\alpha = \partial\mathbf{x}/\partial x^\alpha$, the mapped basis (lattice) vectors are

$$\mathbf{d}_\alpha = \mathbf{A}\mathbf{c}_\alpha = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}\mathbf{c}_\alpha = \mathbf{y}_{,\alpha}.$$

Therefore, since $\mathbf{y}_{,\alpha\beta} = \mathbf{y}_{,\beta\alpha}$ in any coordinate system, from Eq. (10)

$$\Gamma^{\gamma}_{\alpha\beta} = \mathbf{d}^{\gamma} \cdot \mathbf{d}_{\alpha,\,\beta} = \mathbf{d}^{\gamma} \cdot (\mathbf{A}\mathbf{c}_{\alpha})_{,\beta} = \mathbf{d}^{\gamma} \cdot \mathbf{y}_{,\alpha\beta} = \mathbf{d}^{\gamma} \cdot \mathbf{y}_{,\beta\alpha} = \Gamma^{\gamma}_{\beta\alpha}. \tag{13}$$

Hence, the connection is symmetric and also $\mathbf{d}_{\alpha,\,\beta} = \mathbf{d}_{\beta\,,\alpha}$ or $(\mathbf{A}\mathbf{c}_{\alpha})_{,\beta} = (\mathbf{A}\mathbf{c}_{\beta})_{,\alpha}$, which in Cartesian components is equivalent to Eq. (4).

To establish a converse result, albeit only a local one and with the additional requirement that the field $\mathbf{A}$ is *twice* continuously differentiable on K, let us assume that the connection is symmetric. The smoothness of $\mathbf{A}$ implies that the mixed components of the *curvature tensor* $\mathbf{R}$ of the *connection* $\Gamma^{\gamma}_{\alpha\beta}$ vanish, i.e.

$$R_{\cdot\mu\beta\gamma}^{\alpha} = \Gamma^{\alpha}_{\mu\beta,\,\gamma} - \Gamma^{\alpha}_{\mu\gamma,\,\beta} + \Gamma^{\alpha}_{\upsilon\gamma}\Gamma^{\upsilon}_{\mu\beta} - \Gamma^{\alpha}_{\upsilon\beta}\Gamma^{\upsilon}_{\mu\gamma} = 0 \tag{14}$$

which is a direct implication of $\mathbf{d}_{\alpha,\,\beta\gamma} = \mathbf{d}_{\alpha,\,\gamma\beta}$ and the invertibility of $\mathbf{A}$. (Note that defining the curvature tensor does not imply the existence of a metric consistent with it nor, in general, are $\Gamma^{\gamma}_{\alpha\beta}$ the components of the Christoffel symbol of the second kind.) Since the connection is symmetric on K, i.e. $\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha}$, and $\mathbf{R} = \mathbf{0}$, a theorem in differential geometry (see, e.g., Sokolnikoff, 1951, Section 39, pp. 92–96) can be utilized to construct a local deformation $\mathbf{y}$ such that[1]

[1] The foregoing theorem asserts that if $\mathbf{R} = \mathbf{0}$ and the connection is symmetric on K, i.e., $\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha}$, then for every point $\mathbf{z}$ of K there exists a coordinate system $\{\breve{x}^{\alpha}\}$ and an open neighborhood U containing $\mathbf{z}$ such that

$$\breve{\Gamma}^{\gamma}_{\alpha\beta} = 0 \quad \text{on } U.$$

Consequently $\breve{\mathbf{d}}_{\alpha,\,\beta} = 0$ which implies $\breve{\mathbf{d}}_{\alpha}$ is a constant vector $\mathbf{m}_{\alpha}$ in U. Now consider the deformation of U (represented as a field of position vectors relative to an arbitrarily chosen origin) given by

$$\mathbf{y} = \breve{x}^{\alpha}(\mathbf{x})\mathbf{m}_{\alpha}.$$

Clearly,

$$\left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)\breve{\mathbf{c}}_{\beta} = \mathbf{y}_{,\beta} = \mathbf{m}_{\beta} = \breve{\mathbf{d}}_{\beta} = \mathbf{A}\breve{\mathbf{c}}_{\beta},$$

and, therefore, we have shown that if the connection Γ is symmetric (which is a property of a connection independent of coordinate systems), then for every point $\mathbf{z}$ of K it is possible to construct a local deformation $\mathbf{y}$ such that $\mathbf{A} = \partial\mathbf{y}/\partial\mathbf{x}$ locally.

The proof given by Sokolnikoff (1951) does not prove the local invertibility ($\det(\partial\breve{x}^{\alpha}/\partial x^{\beta}) \neq 0$) of the constructed system $\{\breve{x}^{\alpha}\}$, a property essential for it to be considered a coordinate system. For a Riemannian geometry, e.g. the problem arising from the compatibility of a prescribed right Cauchy–Green strain field, the local invertibility can be established globally on simply connected domains by using the property of preservation of angles between vector fields under parallel transport. For a non-Riemannian geometry, i.e. in the absence of a metric, we have been able to establish local invertibility only locally, even on simply connected domains.

It may be worthwhile to mention here that the geometric difference in the problem of right Cauchy–Green compatibility and that of deformation-gradient compatibility lies in the fact that the former is a problem in Riemannian geometry where the connection is symmetric and the main issue is the vanishing of the curvature while the latter is a problem in affine geometry where the vanishing of the curvature is guaranteed but the symmetry of the connection assumes primary importance (also see Acharya and Bassani, 1995).

$$\mathbf{A} = \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \text{ locally.}$$

The geometric proof states that if the tensor field **A** is twice continuously differentiable, in which case the curvature tensor vanishes, the symmetry in the lower indices of the connection, Eq. (10), associated with **A** is equivalent to local compatibility of the tensor field **A**. In Section 5.1, we proved that the assumption of twice differentiability (and hence vanishing curvature) is unnecessary. Even when the field **A** is only continuously differentiable, symmetry of the connection associated with **A** is actually equivalent to global compatibility (and hence local compatibility) of **A**.

To make a connection with the result in Section 5.1, choose $\mathbf{c}_i = \mathbf{e}_i$ and x^i to define a Cartesian coordinate system and note from Eqs. (8) and (9) that $d_{\cdot j}^{i} = A_{\cdot j}^{i}$. Then

$$A_{\cdot j,\,k}^{i} = \Gamma_{jk}^{l} d_{\cdot l}^{i}$$

With the invertibility of $A_{\cdot j}^{i}$ and Eq. (11), it can now be shown that Eq. (4) is equivalent to the symmetry of the connection in any coordinate system, i.e. $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$ is equivalent to $\Gamma_{\alpha\beta}^{\gamma} = \Gamma_{\beta\alpha}^{\gamma}$.

5.3. The torsion tensor

In continuing the geometric argument, we note that although a linear connection is not a tensor, its antisymmetric components (in the lower indices) are the mixed components of a tensor, with respect to the $\mathbf{c}_\alpha$ basis and its reciprocal basis $\mathbf{c}^\alpha$, called the torsion of the connection. Let

$$T_{\alpha\beta}^{\gamma} = \Gamma_{\alpha\beta}^{\gamma} - \Gamma_{\beta\alpha}^{\gamma}. \tag{15}$$

Then the third-order *torsion tensor* of Cartan is

$$\mathbf{T} = T_{\alpha\beta}^{\gamma} \mathbf{c}_\gamma \otimes \mathbf{c}^\alpha \otimes \mathbf{c}^\beta. \tag{16}$$

Note that if a connection is symmetric, then its torsion necessarily vanishes; the converse also holds. If, in a Cartesian coordinate system, $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$, then $\mathbf{T} = \mathbf{0}$, i.e. the torsion vanishes, and α in Eq. (6) also vanishes. Therefore, the non-vanishing torsion of the connection associated with the mapping (or deformation) **A** is a natural measure of incompatibility. In the next subsection we will establish the component-independent property of the field **A** associated with compatibility and provide a useful formula for computing the torsion tensor.

Finally we note that in geometric terminology, a vanishing torsion, $\mathbf{T} = \mathbf{0}$, and a vanishing curvature, $\mathbf{R} = \mathbf{0}$ with its components given in Eq. (14), would make the associated mathematical construct a locally Euclidean affine geometry. Even though these properties alone allow the construction of a local Cartesian coordinate system on the manifold (as illustrated in the outline of the proof of compatibility in this section), it is still not simply Euclidean since no notion of a metric is defined with the geometry, i.e. it is not Riemannian. In the setting of incompatibility, i.e. a non-symmetric connection, the geometry is, of course, non-Riemannian.

5.4. A direct representation of compatibility

We have proven that a symmetric connection, i.e. a vanishing torsion tensor, associated with the continuously differentiable field $\mathbf{A}$ (which may not be twice continuously differentiable) is equivalent to global (local) compatibility of $\mathbf{A}$ on a simply connected domain. In this section we obtain another property of the field $\mathbf{A}$, in component-independent terms without involving a basis or lattice vectors, that characterizes the symmetry of the connection components (or equivalently the symmetry reflected in $A^{\cdot i}_{j,k} = A^{\cdot i}_{k,j}$).

From the definition of the connection components $\Gamma^{\gamma}_{\alpha\beta}$ and $\mathbf{d}_\alpha$ we know that

$$\Gamma^{\gamma}_{\alpha\beta} - \Gamma^{\gamma}_{\beta\alpha} = \mathbf{d}^{\gamma} \cdot \left[\mathbf{d}_{\alpha,\beta} - \mathbf{d}_{\beta,\alpha}\right] = \mathbf{d}^{\gamma} \cdot \left[(\mathbf{A}\mathbf{c}_\alpha)_{,\beta} - (\mathbf{A}\mathbf{c}_\beta)_{,\alpha}\right]$$

$$= \mathbf{d}^{\gamma} \cdot \left[\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{c}_\beta\right)\mathbf{c}_\alpha - \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{c}_\alpha\right)\mathbf{c}_\beta + \mathbf{A}(\mathbf{c}_{\alpha,\beta} - \mathbf{c}_{\beta,\alpha})\right] \tag{17}$$

Therefore, since $\mathbf{c}_\alpha$, $\beta = \mathbf{c}_\beta$, α and $\mathbf{d}^\gamma$ is a basis, the symmetry of the connection, i.e., $\Gamma^{\gamma}_{\alpha\beta} - \Gamma^{\gamma}_{\beta\alpha} = 0$ is equivalent to

$$\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{c}_\beta\right)\mathbf{c}_\alpha = \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{c}_\alpha\right)\mathbf{c}_\beta. \tag{18a}$$

Now, let $\mathbf{v} = v^\alpha \mathbf{c}_\alpha$ and $\mathbf{u} = u^\beta \mathbf{c}_\beta$ be two arbitrary vectors. If Eq. (18a) holds, then

$$\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{v}\right)\mathbf{u} = v^\alpha u^\beta\left[\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{c}_\alpha\right)\mathbf{c}_\beta\right] = v^\alpha u^\beta\left[\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{c}_\beta\right)\mathbf{c}_\alpha\right] = \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{u}\right)\mathbf{v} \quad \textit{for all } \mathbf{u}, \mathbf{v}. \tag{18b}$$

The converse of the previous statement follows directly: Eq. (18b) implies Eq. (18a) which, from Eq. (17), implies $\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha}$. Hence,

$$\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha} \tag{19}$$

and

$$\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{v}\right)\mathbf{u} = \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\mathbf{u}\right)\mathbf{v} \quad \text{for all } \mathbf{u}, \mathbf{v} \tag{20}$$

are *equivalent statements of compatibility*. From Eqs. (15), (16), and (19), so is $\mathbf{T} = \mathbf{0}$.

We now give another demonstration of the equivalence of $A^{\cdot i}_{j,k} = A^{\cdot i}_{k,j}$ and

$\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha}$, where, as before, $A_{\cdot j}^{i} = \mathbf{e}^i \cdot \mathbf{A}\mathbf{e}_j$ are the rectangular Cartesian components of $\mathbf{A}$. Since

$$A_{\cdot j,\,k}^{i} - A_{\cdot k,\,j}^{i} = \mathbf{e}^i \cdot \left[\left(\frac{\partial A}{\partial x} \mathbf{e}_k \right) \mathbf{e}_j - \left(\frac{\partial A}{\partial x} \mathbf{e}_j \right) \mathbf{e}_k \right],$$

it follows that $\mathbf{A}_{\cdot j}^{i}, k = A_{\cdot k}^{i}, j$ is equivalent to

$$\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} \mathbf{e}_k \right) \mathbf{e}_j = \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} \mathbf{e}_j \right) \mathbf{e}_k,$$

since $\mathbf{e}_k$ is a basis. Now, using similar arguments as in the case of the symmetric connection, we find that $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$ is equivalent to Eq. (20) and, therefore, also is equivalent to $\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha}$.

Having established that Eq. (20) is equivalent to $\Gamma^{\gamma}_{\alpha\beta} = \Gamma^{\gamma}_{\beta\alpha}$ and $A_{\cdot j,\,k}^{i} = A_{\cdot k,\,j}^{i}$, we now define a tensor that reflects the incompatibility inherent in the field $\mathbf{A}$. Consider any third-order tensor $\mathbf{B}$ and two bases $\{\mathbf{g}_i\}$ and $\{\mathbf{h}_i\}$. Define the components of $\mathbf{B}$ by

$$B^{ijk} = \mathbf{g}^i \cdot \left[(\mathbf{B}\mathbf{h}^k)\mathbf{h}^j \right], \tag{21a}$$

so that $\mathbf{B}$ has the representation

$$\mathbf{B} = B^{ijk} \mathbf{g}_i \otimes \mathbf{h}_j \otimes \boldsymbol{h}_k. \tag{21b}$$

Now define the tensors $\hat{\mathbf{B}}$ and $\mathbf{B}_{\mathrm{skw}}$ by, respectively,

$$\hat{\mathbf{B}} = B^{ikj} \mathbf{g}_i \otimes \mathbf{h}_j \otimes \mathbf{h}_k \tag{21c}$$

$$\mathbf{B}_{\mathrm{skw}} = \mathbf{B} - \hat{\mathbf{B}}. \tag{21d}$$

(It is easy to see that given $\mathbf{B}$, the definition of $\hat{\mathbf{B}}$ is unique, regardless of the bases chosen to define it.) With the definitions (21), it is again easy to see that the assertion

$$(\mathbf{B}\mathbf{v})\mathbf{u} = (\mathbf{B}\mathbf{u})\mathbf{v} \quad \text{for all } \mathbf{u}, \mathbf{v} \tag{22}$$

is equivalent to

$$\mathbf{B}_{\mathrm{skw}} = \mathbf{0}. \tag{23}$$

Hence, we adopt the field represented by the skew-symmetric part of the gradient field of $\mathbf{A}$ as a measure of the incompatibility of $\mathbf{A}$, i.e.

$$\boldsymbol{\Lambda} \equiv \left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}} \right)_{\mathrm{skw}}. \tag{24}$$

From Eqs. (19)–(24), if $\boldsymbol{\Lambda} = \mathbf{0}$ then $\mathbf{A}$ is compatible. As shown in Appendix B, the torsion tensor (16) is simply a pull-back, to the configuration K, of $(\partial\mathbf{A}/\partial\mathbf{x})_{\text{skw}}$:[2]

$$\mathbf{T} = \mathbf{A}^{-1}\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)_{\text{skw}} = \mathbf{A}^{-1}\boldsymbol{\Lambda}. \tag{25}$$

Finally, since $\Lambda_{\cdot jk}^{i} = A_{\cdot j}^{i}, k - A_{\cdot k}^{i}, j$, we note from Eq. (6) that

$$\alpha^{ip} = -\frac{1}{2}e^{pjk}\Lambda_{\cdot jk}^{i}. \tag{26}$$

6. Local incompatibility and the presence of defects

In this Section we make a connection between the presence of geometrically necessary dislocations in C and non-vanishing torsion related to $\mathbf{F}^{e-1}$. Also, the relationship of the lattice incompatibility, characterized by the presence of torsion related to $\mathbf{F}^{e}$, to a lattice containing defects is illustrated by considering a crystal deforming in single slip. By the term 'geometrically-necessary dislocations' we understand the definition set forth in Section 5 in the discussion surrounding Eqs. (7a) and (7b). This Section concludes with results for multiple slip under small-strain kinematics.

We begin with the observation that if there does not exist an excess of dislocation lines of one sign piercing any surface element of C then the cumulative Burgers vector of the dislocations enclosed in the loop of any closed curve in C is the zero vector. Using Eq. (7), the previous assertion can be readily shown to be equivalent to the symmetry in certain indices of the derivative, with respect to coordinates, of the rectangular Cartesian components of the tensor $\mathbf{F}^{e-1}$, i.e. $F_{ij,\,k}^{e-1} = F_{ik,\,j}^{e-1}$. Hence, asymmetry in these components of the derivatives of the rectangular Cartesian components of $\mathbf{F}^{e-1}$ at any point of C is equivalent to the presence of geometrically necessary dislocations. Clearly, then, a non-vanishing $(\partial\mathbf{F}^{e-1}/\partial\mathbf{x})_{\text{skw}}$ or non- vanishing torsion associated with $\mathbf{F}^{e-1}$ is also equivalent to the presence of geometrically necessary dislocations in C as demonstrated in Section 5.

In order to relate the notions of geometrically necessary dislocations and incompatibility, we note from the result of the analytical argument that local incompatibility of $\mathbf{F}^{e-1}$ around a point $\mathbf{x}$ in C (i.e., the existence of $\mathbf{x}$ in C around which there is no neighborhood where a deformation compatible with $\mathbf{F}^{e-1}$ can be envisaged) is equivalent to $F_{ij,\,k}^{e-1} \neq F_{ik,\,j}^{e-1}$ at that point. Hence we now find that

[2] In the definition of $(\partial\mathbf{A}/\partial\mathbf{x})_{\text{skw}}$ we have taken full advantage of the fact that the domain and range of $\mathbf{A}(\mathbf{x})$ are identical inner-product spaces. Therefore, it is not necessary to be particular about the co-variant-contravariant nature of $(\partial\mathbf{A}/\partial\mathbf{x})_{\text{skw}}$ or the choice of the bases used to define it. While unnecessary for the current purpose, it is an easy matter to adjust the definition of $(\partial\mathbf{A}/\partial\mathbf{x})_{\text{skw}}$ in order for Eq. (25) to make sense even when the tensor field $\mathbf{A}$ is conceived as a two-point tensor between two general manifolds whose tangent spaces at corresponding points are not equipped with a metric.

local incompatibility of $\mathbf{F}^{e-1}$, *non-vanishing* $(\partial \mathbf{F}^{e-1}/\partial \mathbf{x})_{skw}$, *non-vanishing torsion associated with* $\mathbf{F}^{e-1}$, *and the presence of geometrically necessary dislocations in* C are all equivalent notions.

6.1. Mapping of infinitesimal parallelograms

To understand the implications of the incompatibility of $\mathbf{F}^e$ on R, we note that Eq. (20), with the field in question being $\mathbf{F}^e$ and the gradient referring to a referential one, is equivalent to the compatibility of $\mathbf{F}^e$ on R. The mapping of a parallelogram in R, with a vertex at point $\mathring{\mathbf{X}}$ and edge vectors $\mathbf{v}$ and $\mathbf{u}$, is characterized by

$$\frac{\partial \mathbf{F}^e}{\partial \mathbf{X}}(\mathring{\mathbf{X}})\mathbf{v} = \mathbf{F}^e(\mathring{\mathbf{X}} + \mathbf{v}) - \mathbf{F}^e(\mathring{\mathbf{X}}) + o(|\mathbf{v}|), \tag{27a}$$

$$\frac{\partial \mathbf{F}^e}{\partial \mathbf{X}}(\mathring{\mathbf{X}})\mathbf{u} = \mathbf{F}^e(\mathring{\mathbf{X}} + \mathbf{u}) - \mathbf{F}^e(\mathring{\mathbf{X}}) + o(|\mathbf{u}|). \tag{27b}$$

On neglecting higher order terms in Eq. (27), compatibility as expressed in Eq. (20) implies

$$\mathbf{F}^e(\mathring{\mathbf{X}})\mathbf{v} + \mathbf{F}^e(\mathring{\mathbf{X}} + \mathbf{v})\mathbf{u} = \mathbf{F}^e(\mathring{\mathbf{X}})\mathbf{u} + \mathbf{F}^e(\mathring{\mathbf{X}} + \mathbf{u})\mathbf{v},$$

i.e. the images of all infinitesimal parallelograms in the reference close under a compatible mapping.

Due to the equivalence of the notion of compatibility with Eq. (20), it is also true that when $\mathbf{A}$ is incompatible on R, there is a pair of infinitesimal vectors in R for which an infinitesimal parallelogram does not close under mapping by $\mathbf{A}$. The lattice vectors can be considered as vectors of R if such vectors are mapped by $\mathbf{F}^e$; with this interpretation in mind, we find that the image of a 'small' parallelogram drawn on the reference lattice, whose characteristic dimension is larger than the scale at which the field $\mathbf{F}^e$ is homogeneous on R, may not close when the field $\mathbf{F}^e$ is incompatible on R. Thus, the image lattice under such a mapping appears to be disconnected, implying the presence of defects in it.

6.2. Incompatibility and single slip

We now examine the manifestation of incompatibility, in the sense of this paper, within the constitutive structure of crystal plasticity. We consider two cases of an identical shearing-type overall motion of a body with the difference being in the orientation of the slip system. These examples illustrate the nature of the incompatibility of the intermediate configuration and the deformed lattice that result in the cases of slip parallel and perpendicular to the overall shearing. We simply consider the elasto-plastic kinematics of the problem, and the motions that will be considered can be thought of as physically realizable under suitable body force fields.

We choose a rectangular Cartesian coordinate system with base vectors $\mathbf{e}_i$ and denote the reference placement of points by their coordinates X_i and the current placement by the coordinates x_i. The overall motion being considered has the description

$$x_1 = \kappa(X_2, t) + X_1,$$

$$x_2 = X_2,$$

$$x_3 = X_3, \tag{28a}$$

with deformation gradient

$$\mathbf{F} = \mathbf{I} + \kappa_{,2}\mathbf{e}_1 \otimes \mathbf{e}_2, \tag{28b}$$

where $\mathbf{I}$ denotes the identity tensor.

Since the description of the motion varies only with the X_2 coordinate at each instant of time, therefore the history of the motion of the body up to any time also varies only with the X_2 coordinate. This implies that all constitutively dependent quantities also vary only with the X_2 coordinate. Hence

$$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial X_j}\frac{\partial X_j}{\partial x_i} = \frac{\partial}{\partial X_2}\frac{\partial X_2}{\partial x_i} = \frac{\partial}{\partial X_2}\delta_{2i}$$

6.2.1. Slip parallel to direction of overall shearing

Consider slip in the direction $\mathbf{m}_0 = \mathbf{e}_1$ on slip planes whose normals point in the direction $\mathbf{n}_0 = \mathbf{e}_2$. Since we are considering single slip

$$\mathbf{F} = \mathbf{I} + \kappa_{,2}\mathbf{m}_0 \otimes \mathbf{n}_0,$$

$$\mathbf{F}^{\mathrm{p}} = \mathbf{I} + \gamma\mathbf{m}_0 \otimes \mathbf{n}_0,$$

$$\mathbf{F}^{\mathrm{e}} = \mathbf{I} + (\kappa_{,2} - \gamma)\mathbf{m}_0 \otimes \mathbf{n}_0,$$

$$\mathbf{F}^{\mathrm{e}-1} = \mathbf{I} + (\gamma - \kappa_{,2})\mathbf{m}_0 \otimes \mathbf{n}_0. \tag{29}$$

Now, with κ and γ varying spatially only with respect to $X_2 = x_2$, from Eq. (29)

$$\left(\frac{\partial \mathbf{F}^{e-1}}{\partial \mathbf{x}}\right)_{ijk} = \frac{\partial F^{e-1}_{ij}}{\partial x_k} = \delta_{k2}(\gamma - \kappa_{,2})_{,2}(m_0)_i(n_0)_j = (n_0)_k(\gamma - \kappa_{,2})_{,2}(m_0)_i(n_0)_j$$
$$= \left(\frac{\partial \mathbf{F}^{e-1}}{\partial \mathbf{x}}\right)_{ikj}$$

and

$$\left(\frac{\partial \mathbf{F}^{e}}{\partial \mathbf{X}}\right)_{ijk} = \frac{\partial F^{e}_{ij}}{\partial X_k} = -\delta_{k2}(\gamma - \kappa_{,2})_{,2}(m_0)_i(n_0)_j = -(n_0)_k(\gamma - \kappa_{,2})_{,2}(m_0)_i(n_0)_j$$
$$= \left(\frac{\partial \mathbf{F}^{e}}{\partial \mathbf{X}}\right)_{ikj}$$

Hence, the tensors of incompatibility, $(\partial \mathbf{F}^{e-1}/\partial \mathbf{x})_{skw}$ and $(\partial \mathbf{F}^{e}/\partial \mathbf{x})_{skw}$, vanish.

Thus, for single slip parallel to the direction of overall shearing, the intermediate configuration and the deformed lattice are compatible images of C and the reference lattice, respectively.

6.2.2. Slip perpendicular to direction of overall shearing

Consider slip in the direction $\mathbf{m}_0 = \mathbf{e}_2$ on slip planes whose normals point in the direction $\mathbf{n}_0 = \mathbf{e}_1$. In this case we have

$$\mathbf{F} = \mathbf{I} + \kappa_{,2}\mathbf{n}_0 \otimes \mathbf{m}_0,$$

$$\mathbf{F}^{p} = \mathbf{I} + \gamma\mathbf{m}_0 \otimes \mathbf{n}_0,$$

$$\mathbf{F}^{e} = \mathbf{I} - \gamma\mathbf{m}_0 \otimes \mathbf{n}_0 + \kappa_{,2}\mathbf{n}_0 \otimes \mathbf{m}_0 - \gamma\kappa_{,2}\mathbf{n}_0 \otimes \mathbf{n}_0,$$

$$\mathbf{F}^{e-1} = \mathbf{I} - \kappa_{,2}\mathbf{n}_0 \otimes \mathbf{m}_0 + \gamma\mathbf{m}_0 \otimes \mathbf{n}_0 - \gamma\kappa_{,2}\mathbf{m}_0 \otimes \mathbf{m}_0. \tag{30}$$

Therefore, from Eq. (30),

$$\left(\frac{\partial \mathbf{F}^{e-1}}{\partial \mathbf{x}}\right)_{ijk} = \frac{\partial F^{e-1}_{ij}}{\partial x_k}$$
$$= (m_0)_k\left[-\kappa_{,22}(n_0)_i(m_0)_j + \gamma_{,2}(m_0)_i(n_0)_j - (\gamma\kappa_{,2})_{,2}(m_0)_i(m_0)_j\right], \tag{31a}$$

$$\left(\frac{\partial \mathbf{F}^{e}}{\partial \mathbf{X}}\right)_{ijk} = \frac{\partial F^{e}_{ij}}{\partial X_k}$$
$$= (m_0)_k\left[\kappa_{,22}(n_0)_i(m_0)_j + \gamma_{,2}(m_0)_i(n_0)_j - (\gamma\kappa_{,2})_{,2}(m_0)_i(m_0)_j\right], \tag{31b}$$

and, hence, we have a non vanishing incompatibility because of the asymmetry in j and k of the second terms of the right-hand sides of both Eqs. (31a) and

(31b), i.e. $(\partial \mathbf{F}^{e-1}/\partial \mathbf{x})_{skw} \neq \mathbf{0}$ and $(\partial \mathbf{F}^{e}/\partial \mathbf{X})_{skw} \neq \mathbf{0}$. In terms of the field $\mathbf{F}^{e-1} \equiv \mathbf{A}$ with Eqs. (30) and (31), the three measures of incompatibility Eqs. (24)–(26) are:

$$\mathbf{\Lambda} = \left(\frac{\partial \mathbf{F}^{e-1}}{\partial \mathbf{x}}\right)_{skw} = \gamma_{,2}\mathbf{m}_0 \otimes (\mathbf{n}_0 \otimes \mathbf{m}_0 - \mathbf{m}_0 \otimes \mathbf{n}_0), \tag{32a}$$

$$\mathbf{T} = \mathbf{F}^{e}\left(\frac{\partial \mathbf{F}^{e-1}}{\partial \mathbf{x}}\right)_{skw} = \gamma_{,2}(\mathbf{m}_0 + \kappa_{,2}\mathbf{n}_0) \otimes (\mathbf{n}_0 \otimes \mathbf{m}_0 - \mathbf{m}_0 \otimes \mathbf{n}_0), \tag{32b}$$

$$\alpha^{ip} = -\gamma_{,2}\mathrm{e}^{pjk}(m_0)_i(n_0)_j(m_0)_k, \tag{32c}$$

and with $\mathbf{m}_0 = \mathbf{e}_2$ and $\mathbf{n}_0 = \mathbf{e}_1$ the only nonzero component of $\boldsymbol{\alpha}$ is $\alpha_{23} = -\gamma_{,2}$.

Thus, the slip geometry in this case, i.e. perpendicular to the overall shearing, induces an incompatible intermediate configuration and deformed lattice. This is generally the case unless slip is parallel to the overall shearing.

6.2.3. Multiple slip and incompatibility under small strains

Whereas under single slip one can represent $\mathbf{F}^{p}$ directly in terms of γ as given in Eq. (29) or (30), under multiple slip at finite deformations this is not possible; athough $\mathbf{L}^{p}$ given in Eq. (2) is expressed as a linear combination involving the slip rates on all systems, neither $\mathbf{F}^{p}$ nor $\mathbf{F}^{p-1}$ can be written as a sum involving the total slips. In the setting of small strains (see, e.g., Hutchinson, 1970; Fleck et al., 1994), the total displacement gradient is taken to be the sum of elastic and plastic parts:

$$u_{i,j} = U^{e}_{ij} + U^{p}_{ij}, \tag{33}$$

where the symmetric parts form the corresponding components of total, elastic, and plastic strains, ε_{ij}, ε^{e}_{ij} and ε^{p}_{ij}, respectively. The plastic part of the displacement gradient is taken to arise solely from slips γ^{κ} on all systems ($\kappa = 1, N$) according to

$$U^{p}_{ij} = \sum_{\kappa}\gamma^{\kappa}m^{\kappa}_i n^{\kappa}_j, \tag{34}$$

where, as before, the unit vectors $\mathbf{m}^{\kappa}$ and $\mathbf{n}^{\kappa}$, respectively, denote the slip direction and slip-plane normal for system κ.

Now, following the analysis of Section 5.1, the plastic part of the displacement gradient, and hence also the elastic part of the displacement gradient, are incompatible if

$$\alpha_{il} = e_{lkj}U^{p}_{ij,k} \neq 0.$$

Substituting Eq. (34) for in $\mathbf{U}^{p}$ the previous expression one obtains Nye's dislocation density tensor

$$\alpha_{il} = e_{lkj} \sum_{\kappa} \gamma^{\kappa}_{,k} m^{\kappa}_i n^{\kappa}_j. \tag{35}$$

One can immediately see that gradients of slip on a given system that are in the direction of the normal to that slip plane (i.e. $\nabla\gamma^{\kappa}$ parallel to $\mathbf{n}^{\kappa}$) give no contribution to the sum in Eq. (35). Note also that since the total displacement gradient is compatible, from Eq. (33) $e_{lkj} U^{\mathrm{e}}_{ij}, k = -e_{lkj} U^{\mathrm{p}}_{ij}, k$.

We close this section with the following, important observation that has implications when incorporating the effects of lattice incompatibility into single crystal constitutive relations as discussed in the next section. In either setting of finite or infinitesimal kinematics, incompatibility is a property that most naturally arises in terms of quantities like $\boldsymbol{F}^{\mathrm{e}}$ or $\boldsymbol{U}^{\mathrm{e}}$ (or $\boldsymbol{U}^{\mathrm{e}}$), respectively, for reasons discussed in Section 4, at the end of Section 5.1, and in this section. For small strains, it is tempting to associate the contribution $\gamma^{\kappa}_{,k} m^{\kappa}_i n^{\kappa}_j$ to the summation in Eq. (35) with the incompatibility of slip system κ, but this is only a consequence of the algebraic structure of the dislocation density tensor (incompatibility measure) and cannot be justified on physical grounds. For example, one can contemplate a situation where $\boldsymbol{\alpha}$ vanishes under multiple slip even though there are nonzero contributions to the summation which cancel. In other words, lattice incompatibility can be relieved through the activation of secondary slip systems. Finally, we mention another possibility, motivated by Eq. (7b) with the term in the integrand multiplying r_p associated with α_{ip} and S taken to be a slip plane, say slip plane κ (also see the discussion following Eq. (7b)). Then the integral (Eq. (7b)) gives the cumulative Burgers vector of all dislocation lines piercing that plane, and one could take the integrand $\alpha_{ip} n^{\kappa}_p$, as a measure of the incompatibility associated with slip system κ.

7. Incompatibility, instantaneous hardening, and the BVP of incremental equilibrium

The effects of lattice incompatibility can naturally lead to a gradient-type, nonlocal constitutive framework for single crystals (or for any material system where the total deformation is made up of parts which are not constrained to be individually compatible). There are several approaches which can be taken, and have been taken in various settings, depending on whether the formulation is rate independent or rate dependent and on whether so-called higher-order stresses are introduced. The formulation outlined below is based upon the *simple theory* proposed by Acharya and Bassani (1995) where a particular strain gradient, which is taken to be a measure of elastic (or plastic) incompatibility, enters the flow rules *only* through the instantaneous hardening-rate. With this approach, one can readily adopt either a rate independent or rate dependent point of view. Furthermore, this simple theory preserves the classical structure of the rate-independent incremental boundary-value problems

(Hill, 1958) and does not require higher-order stresses or additional boundary conditions as in, for example, the Fleck and Hutchinson (1993) theory.

Given a number of now well-known size-scale phenomena arising in plastic flow such as those mentioned in the introduction — with the commonly observed trend that *smaller is harder* — we work with the hypothesis that this incompatibility directly influences the hardening behavior. Since lattice incompatibility is characterized by a spatial gradient of the elastic deformation field (or its inverse), when incorporated in the hardening response a material length-scale must enter the theory on dimensional grounds. Consistent with the physical motivation for the significance of lattice incompatibility that has formed the basis of this paper, in what follows we will focus on single crystal formulations, although an even simpler J_2 flow theory-type constitutive framework has been proposed by Acharya and Bassani (1996) and applied by Acharya et al. (1999) and Luo (1998).

With this motivation in mind, it seems natural to incorporate the effects of incompatibility of the lattice or the intermediate configuration in the hardening response of a single crystal. When the conventional hyperelastic stress response is retained, perhaps the most immediate and natural modification of conventional hardening constitutive hypotheses (see, e.g., Bassani, 1994) is given by

$$\dot{\tau}^{\kappa}_{\mathrm{cr}} = \sum_{\eta} h^{\kappa\eta}\left(\{\gamma^{\mu}\},\mathbf{G}\right)\dot{\gamma}^{\eta}, \tag{36}$$

where $h^{\kappa\eta}$ is the hardening matrix, $\mathbf{G}$ is an appropriate frame-indifferent measure of the incompatibility, and γ^{κ} and $\tau^{\kappa}_{\mathrm{cr}}$ are the crystallographic slips and critical stresses, respectively, on the κth slip system (the choice of the critical shear stresses instead of the crystallographic slips as dependencies of the hardening matrix does not alter the essential feature of this discussion). In a rate-independent setting where a slip system is said to be active if and only if $\tau^{\kappa} = \tau^{\kappa}_{\mathrm{cr}}$ and $\dot{\tau}^{\kappa} = \dot{\tau}^{\kappa}_{\mathrm{cr}}$ ($\tau^{\kappa} = \mathbf{m}^{\kappa} \cdot (\boldsymbol{\sigma}\mathbf{n}^{k})$, where $\boldsymbol{\sigma}$ is the Cauchy stress tensor), such a constitutive proposal has some highly desirable properties with regard to the formulation of the boundary-value problems (bvp) of incremental equilibrium. These properties also hold in a rate-dependent setting, e.g. where $\dot{\gamma}^{\kappa} = f(\tau^{\kappa})$.

First and foremost, the abovementioned modification introduces a physically motivated constitutive length-scale in the definition of the rate-independent material, purely on mechanical grounds. The stress-rate response of the material remains, as in the conventional gradient-independent case, a homogeneous function of degree one in a suitable strain-rate measure; hence, all classical features of the definition of the bvp remain unaltered as only the incremental moduli, which are only current-state dependent, are altered, and a general dependence of the moduli on the current state is accounted for in the classical theory of the bvp of incremental equilibrium. An important consequence that may be highlighted is the fact that the order of the partial differential equations for the velocities out of a given state remains at two and no extra boundary conditions, over and above the conventional specification, are required to solve the problem.

We note here that while the above comments on well-posedness apply unequivocally for the incremental bvp if the rate equation of equilibrium is considered to be the only balance law governing the mechanical evolution of the body, the situation is not as clear if, instead, the full problem of evolution involving the equilibrium equations, is considered. Whether extra boundary conditions are required in this case with a gradient modification is a difficult, open question. However, if a transition to a true non-local measure (instead of a gradient measure) can be proven to be adequate for the purpose of delivering uniqueness of solutions, then it is an easy matter, both in terms of physical motivation and mathematical ease, to replace a hardening measure like $(\partial \mathbf{A}/\partial \mathbf{x})_{\mathrm{skw}}$ by an area integral of it, say over specific planes of interest and over a physically motivated finite area. Such a measure would have the physical interpretation of characterizing the net Burgers vector of all the dislocations threading the plane in question within the prescribed area.

In terms of the broad qualitative changes in the nature of solutions, it is to be expected that classical results for a bifurcation out of a *homogeneous* state will remain unaltered for rate-independent solids. However, the nature of the solutions will change as soon as inhomogeneous flow sets in, due to the dependence of the incremental moduli on $\mathbf{G}$. Subsequently, plastic flow, after the onset of inhomogeneity, will be nonlocal in the sense that flow at a point is affected by the state of neighboring material points through the hardening moduli.

The abovementioned simplicity in the incremental problem, however, relies crucially on the conventional stress-response not being affected by $\mathbf{G}$. Apart from the fact that such a constitutive assumption is justifiable on grounds of simplicity, there also exists a thermodynamic justification for it.

The need for a material length-scale (through a dependence on higher-order gradients, of a suitable deformation-measure, in material response) in thermally-insensitive plastic constitutive structure arose in trying to resolve certain types of observed phenomena within continuum descriptions that are otherwise adequate for a wide variety of applications. Higher-order stresses are not included in these classical descriptions, while it is known, from the thermodynamic analysis of hyperelastic constitutive asumptions for elastic materials, that higher-gradients of deformation are admissible in material response in the presence of higher-order stresses (Green and Rivlin, 1964), and only in the presence of such (Gurtin, 1965). However, elasto-plastic materials being different from elastic materials due to their significant history-dependence in response, it is perhaps natural to probe whether such materials can accomodate higher deformation-gradient dependencies in response, within the hypothesis that these materials cannot support higher-order stresses. The foregoing fact translates to the mathematical statement of balance of energy for such materials remaining unaltered by any mechanical stress-power term due to higher-order stresses. Working within the confines of this setting, it can be shown (Acharya and Shawki, 1995) that higher deformation-gradient dependencies can be accomodated in the yield and internal-variable rate response of elasto-plastic materials, but a dependence of the free-energy, and consequently the stress response, on the value of such gradients at the current instant of time (as opposed to a dependence on their past history through the current values of the internal variables) is ruled out.

Since the current value of $\mathbf{G}$ is a function of the current values of the deformation gradient and its gradient and of $\mathbf{F}^{\mathrm{p}}$ and its gradient, and since $\mathbf{F}^{\mathrm{p}}$ is invertible, $\mathbf{G}$ cannot affect the stress response if the current value of the second-deformation-gradient is inadmissible. Thus, we find that a conventional elasto-plastic and elasto-viscoplastic stress-response with only a gradient modified slip-hardening rule does not violate any general principle of thermomechanics. In Appendix A, we derive the rotation-invariant versions of the incompatibility measures derived in this paper.

8. Conclusions

This paper has dealt with an analysis of the incompatibility associated with the intermediate configuration of crystal plasticity and a lattice with defects. The kinematical content of the paper establishes results from the theory of continuous distributions of dislocations within the framework of continuum crystal plasticity theory. The inclusion of these incompatibility measures in the conventional constitutive description of crystal plasticity has been achieved on physical and thermodynamic grounds. The implications of the modified constitutive structure with respect to the incremental bvp of equilibrium for rate-independent and rate-dependent response has also been discussed.

The work presented here establishes a physically motivated non-local theory of crystal plasticity. The theory has some desirable properties with regard to the formulation of the boundary value problem of incremental equilibrium in that the conventional specification (order of the problem, boundary conditions) is inherited, without change or additions, in the modified theory. Consequently, all the well- established general results, i.e. those that hold without a commitment to any particular piecewise-linear incremental response, of the conventional theory on uniqueness, bifurcation, and variational and extremum principles remain applicable in the present case. In particular, an important result pertaining to the bifurcation of an incremental solution out of a homogeneous state is retained in its conventional form for rate-independent solids. The suggested constitutive modification is also justified on thermodynamic grounds.

Due to the inclusion of a material parameter with dimensions of length in the hardening response, an intrinsic length-scale is introduced in the theory. Spatial derivatives of elastic deformation enter into material response which, in the case of single slip, at least, make the slip evolution dependent on spatial derivatives of slip. It is hoped that such hardening descriptions may prove successful in explaining patterning of microstructures related to slip activity.

Finally, we mention two recent results that incorporate incompatibility measures into numerical solutions of boundary value problems. The first involves solutions for torsion of small rods and deformations of thin films in an isotropic version of the theory (Luo, 1998). The second are calculations that predict the effect of hard particles on the deformation of single crystals undergoing single slip. The former predict trends in accord with the Fleck et al. (1994) experiments and calculations, and the latter predict trends in accord with the dislocation solutions of Cleveringa et al. (1997). Papers on both analyses are forthcoming.

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Appendix A. Invariance under superposed rigid-body motions

In this section we deduce appropriate measures of the incompatibilities, $(\partial \mathbf{F}^e/\partial \mathbf{X})_{skw}$ and $(\partial \mathbf{F}^{e-1}/\partial \mathbf{x})_{skw}$ in order to render the responses for the critical shear stress-rates on slip planes and the slip increments frame-indifferent.

Let two motions of the body, $\mathbf{x}^+$ and $\mathbf{x}$, be related by

$$\mathbf{x}^+(\mathbf{X}, t) = \mathbf{c}(t) + \mathbf{Q}(t)\{\mathbf{x}(\mathbf{X}, t) - \mathbf{c}(t)\},$$

where $\mathbf{c}$ and $\mathbf{Q}$ are position-vector-valued and orthogonal second-order-tensor valued functions of time, respectively. Let $\mathbf{A}^+$, $\mathbf{B}^+$, $\mathbf{A}$ and $\mathbf{B}$ be time-dependent invertible second-order tensor fields, defined on configurations of the motions $\mathbf{x}^+$ and $\mathbf{x}$, respectively, and let them be related by

$$\mathbf{B}^+(\mathbf{x}^+, t) = \mathbf{Q}(t)\mathbf{B}(\mathbf{x}, t) \quad (\text{e.g., } \mathbf{B} \equiv \mathbf{F}^e)$$

and

$$\mathbf{A}^+(\mathbf{x}^+, t) = \mathbf{A}(\mathbf{x}, t)\mathbf{Q}^\mathbf{T}(t) \quad (\text{e.g., } \mathbf{A} \equiv \mathbf{F}^{e-1}).$$

We now view the configurations of the motions $\mathbf{x}^+$ and $\mathbf{x}$ as being parametrized by a rectangular Cartesian coordinate system and all tensors as expressed in terms of the natural basis $\mathbf{e}_i$ of this coordinate system. Also, we use the notation

$$x^+(\mathbf{x}^+);\quad x^+ = \left(x_1^+, x_2^+, x_3^+\right)$$

$$x(\mathbf{x});\quad x = (x_1, x_2, x_3).$$

to represent the corresponding coordinate maps.

In order to find a representation of the incompatibilities for configurations of the motion $\mathbf{x}^+$ in terms of quantities pertaining to the $\mathbf{x}$ motion and the function $\mathbf{Q}$, we consider

$$A_{km}^+\left(x^+, t\right) = A_{kp}(x, t)Q_{mp}(t),$$

which implies

$$A_{km,\,i}^+\left(x^+, t\right) = A_{kp,\,j}(x, t)Q_{mp}(t)\frac{\partial x_j}{\partial x_i^+}\left(x^+, t\right).$$

But

$$A_{km,\,i}^+ = \mathbf{e}_k\cdot\left(\frac{\partial\mathbf{A}^+}{\partial\mathbf{x}^+}\mathbf{e}_i\right)\mathbf{e}_m = \left(\frac{\partial A^+}{\partial x^+}\right)_{kmi};\quad \frac{\partial x_j}{\partial x_i^+} = \mathbf{e}_j\cdot\frac{\partial\mathbf{x}}{\partial\mathbf{x}^+}\mathbf{e}_i = Q_{ji}^{\mathrm{T}};$$

$$A_{kp,\,j} = \left(\frac{\partial A}{\partial x}\right)_{kpj};$$

consequently,

$$\left(\frac{\partial A^+}{\partial x_{\mathrm{skw}}^+}\right)_{kmi} = \left(\frac{\partial A}{\partial x}\right)_{kpj}\left[Q_{mp}Q_{ij} - Q_{ip}Q_{mj}\right].$$

Consider a field variable Ξ (scalar, tensor) defined by the constitutive function $\Xi_{\mathbf{X}}$ at the material point $\mathbf{X}$ depending on $(\partial\mathbf{A}/\partial\mathbf{x})_{\mathrm{skw}}$ at the current time. Let the invariance requirement of the field Ξ be

$$\Xi(\mathbf{X}, t) = \Xi^+(\mathbf{X}, t)$$

for all t and for all choices of the orthogonal tensor history $\mathbf{Q}$. Then, invariance under superimposed rigid-body motions requires that

$$\Xi_{\mathbf{X}}\left(\mathbf{Q}\mathbf{A}^{-1}, \frac{\partial\mathbf{A}^+}{\partial{\mathbf{x}^+}_{\mathrm{skw}}}\right) = \Xi_{\mathbf{X}}\left(\mathbf{A}^{-1}, \frac{\partial\mathbf{A}}{\partial\mathbf{x}_{\mathrm{skw}}}\right)\quad \text{for all choices of } \mathbf{Q},$$

where the arguments are evaluated at $\mathbf{X}$.

Let the tensor $\mathbf{A}^{-1}\equiv\mathbf{F}^{\mathrm{e}}$ have the polar decomposition $\mathbf{A}^{-1}\equiv\mathbf{F}^{\mathrm{e}} = \mathbf{R}^{\mathrm{e}}\mathbf{U}^{\mathrm{e}}$. Then, making the choice $\mathbf{Q} = \mathbf{R}^{\mathrm{e}^{\mathrm{T}}}$

$$\Xi_X\left(A^{-1}_{rs}, \left(\frac{\partial A}{\partial x_{\rm skw}}\right)_{kmi}\right) = \Xi_{\mathbf{X}}\left(U^{\rm e}_{rs}, \left(\frac{\partial A}{\partial x}\right)_{kpj}\left[R^{\rm e}_{pm}R^{\rm e}_{ji} - R^{\rm e}_{pi}R^{\rm e}_{jm}\right]\right)$$

$$= \Xi_{\mathbf{X}}\left(U^{\rm e}_{rs}, \left(\frac{\partial A}{\partial x_{\rm skw}}\right)_{kpj}\left[R^{\rm e}_{pm}R^{\rm e}_{ji} - R^{\rm e}_{pi}R^{\rm e}_{jm}\right]\right).$$

Conversely, it can be checked that any response function for Ξ at a point $\mathbf{X}$ that depends only on $U^{\rm e}_{rs}$, and $(\partial A/\partial x_{\rm skw})_{kpj}[R^{\rm e}_{pm}R^{\rm e}_{ji} - R^{\rm e}_{pi}R^{\rm e}_{jm}]$ at $\mathbf{X}$ satisfies invariance under superimposed rigid-body motions in the sense that, in such a case, $\Xi(\mathbf{X}, t) = \Xi^+(\mathbf{X}, t)$ for all t.

Since the hardening matrix $h_{\alpha\beta}$ has the same invariance requirement as the field Ξ the measure of incompatibility of $\mathbf{F}^{\rm e-1}$ characterized by

$$\left(\frac{\partial F^{\rm e-1}}{\partial x_{\rm skw}}\right)_{kpj}\left[R^{\rm e}_{pm}R^{\rm e}_{ji} - R^{\rm e}_{pi}R^{\rm e}_{jm}\right]$$

is an appropriate frame-indifferent argument for it. A conceptually similar procedure can be used to deduce the frame-indifference requirement arising out of a dependence of $h_{\alpha\beta}$ on $(\partial\mathbf{F}^{\rm e}/\partial\mathbf{X})_{\rm skw}$. Also, instead of the choice $\mathbf{R}^{\rm e}$, a frame-indifferent measure of incompatibility can also be generated by the use of the rotation tensor $\mathbf{R}$ arising out of the polar decomposition of $\mathbf{F}$.

Appendix B. Demonstration of $\mathbf{T}=\mathbf{A}^{-1}(\frac{\partial\mathbf{A}}{\partial\mathbf{x}})_{\rm skw}$

Consider $\mathbf{A}^{-1}(\frac{\partial\mathbf{A}}{\partial\mathbf{x}})_{\rm skw}$. This is a third-order tensor on $\mathbf{K}$ while $(\frac{\partial\mathbf{A}}{\partial\mathbf{x}})_{\rm skw}$ is a third-order, two-point tensor.

Now, $(\frac{\partial\mathbf{A}}{\partial\mathbf{x}})$ can be expressed as

$$\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right) = \left[\mathbf{d}^\gamma\cdot\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\mathbf{e}_\beta\right)\mathbf{e}_\alpha\right]\mathbf{d}^\gamma\otimes\mathbf{e}^\alpha\otimes\mathbf{e}^\beta.$$

From the definition of the skew part of a third-order tensor (Section 5.4)

$$\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\right)_{\rm skw} = [A_{\rm skw}]^\gamma_{\alpha\beta}\mathbf{d}_\gamma\otimes\mathbf{e}^\alpha\otimes\mathbf{e}^\beta,$$

where

$$[A_{\rm skw}]^\gamma_{\alpha\beta} = \left[\mathbf{d}^\gamma\cdot\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\mathbf{e}_\beta\right)\mathbf{e}_\alpha - \mathbf{d}^\gamma\cdot\left(\frac{\partial\mathbf{A}}{\partial\mathbf{x}}\mathbf{e}_\alpha\right)\mathbf{e}_\beta\right].$$

Noting the relationships $\mathbf{A}=\mathbf{d}_\rho\otimes\mathbf{e}^\rho \Longrightarrow \mathbf{A}^{-1}=\mathbf{e}_\rho\otimes\mathbf{d}^\rho$ and Eqs. (15)–(17),

$$\mathbf{A}^{-1}\left(\frac{\partial \mathbf{A}}{\partial \mathbf{x}}\right)_{\text{skw}} = \left\{\mathbf{e}_\rho \otimes \mathbf{d}^\rho\right\}\left\{[A_{\text{skw}}]^\gamma_{\alpha\beta}\mathbf{d}_\gamma \otimes \mathbf{e}^\alpha \otimes \mathbf{e}^\beta\right\} = [A_{\text{skw}}]^\gamma_{\alpha\beta}\mathbf{e}_\gamma \otimes \mathbf{e}^\alpha \otimes \mathbf{e}^\beta$$

$$= \left[\Gamma^\gamma_{\alpha\beta} - \Gamma^\gamma_{\beta\alpha}\right]\mathbf{e}_\gamma \otimes \mathbf{e}^\alpha \otimes \mathbf{e}^\beta = \mathbf{T}.$$

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