A Dynamical Theory of Structured Solids. I Basic Developments

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A dynamical theory of structured solids. I
Basic developments

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Contents

Based on the well-accepted notion of a Bravais lattice of a crystal at the atomic scale and with particular reference to inelastic behaviour of materials, this paper is concerned with the construction of a macroscopic dynamical theory of solids which incorporates the effect of the presence of the atoms and their arrangements. The theory incorporates a wide variety of microstructural processes occurring at various physical scales and has a range approaching the atomic scale. These processes include the *effect* of the motion of individual dislocations, which are modeled here as continuous distributions at the macroscopic scale.

The formulation of the basic theory, apart from the kinematical and kinetical variables employed in classical continuum mechanics, utilizes a triad of independent

vector-valued variables – called directors – (or an equivalent tensor-valued variable) which represent the lattice vectors and are determined by additional momentum-like balance laws associated with the rate of change of lattice deformation in the spirit of a Cosserat (or directed) continuum. A suitable composition of the triad of directors and the ordinary deformation gradient is identified as a measure of permanent or *plastic* deformation, the referential gradient of which plays a significant role in the kinematics of lattice defects. In particular, a uniquely defined skew-symmetric part of the gradient of plastic deformation is identified as a measure of the density of dislocations in the crystal. The additional momentum-like balance laws associated with the rate of lattice deformation include the effect of forces necessary to maintain the motion of dislocations, as well as the inertia effects on the microscopic and submicroscopic scales arising from the director fields. The basic theoretical developments also provide important clarifications pertaining to the structure of the constitutive response functions for both viscoplasticity and (the more usual) rate-independent plasticity.

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1. Introduction and background

The concept of a crystal based on a Bravais lattice at the atomic scale is used as a basic premise in this paper and a companion one (Part II under the same title) to present a general (macroscopic) dynamical theory of structured solids. The basic theory in Part I is applicable to a wide range of material behaviour, including that of elastic-plastic and elastic-viscoplastic metals. In particular, in the present Part I, attention is focused on the detailed development of constitutive equations for crystal plasticity in the presence of continuously distributed dislocations. The term *crystal plasticity* refers to a particular mode of permanent deformation, say in a single crystal, caused by the movements of the atoms of a crystal with respect to each other that give rise to a rearrangement of their long-range ordering. This movement of the atoms is greatly influenced by the presence of certain imperfections in the ordering of the atoms. These imperfections – called dislocations – can propagate through the crystal, reducing the forces required in maintaining the motion of the atoms relative to each other, and thus facilitating the occurrence of permanent deformation in the crystal.

For certain applications, it is convenient to ignore the details of the atomic nature of dislocations in a crystal and to regard an array of similar dislocations as being distributed uniformly throughout the medium. Using this notion of 'continuous distribution of dislocations', the kinematics of a crystal lattice have been studied by Eshelby (1956), Bilby (1960), Kondo (1952, 1964) and Kröner (1960), among others. However, no satisfactory extension of such studies to incorporate the effects of dislocations explicitly in the characterization of plastic deformation of crystals and their hardening characteristics on a macroscopic scale has been given so far. Experience of the past decade or so suggests that the goal for construction of a satisfactory dynamical theory may be achieved by utilizing a judicious choice of augmented variables via a Cosserat (or directed) continuum. Indeed, some support for such an approach has been mentioned in the literature on dislocations (see, for example, the quotations (*a*), (*b*), (*c*) from Nabarro 1987)[†]. Given this background, in addition to the variables used in classical continuum mechanics, a triad of

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† Direct quotations from Nabarro (1987) and one other relevant reference are listed in Appendix A.

independent vector-valued variables – called directors – is used to represent the effect of lattice vectors (see (2.1)) and are determined by additional momentum-like balance laws for the rate of change of the director fields.

Background information concerning *Cosserat* or '*directed*' continua, which are endowed with one or more directors as additional kinematical variables, can be found in Green *et al.* (1965), Truesdell & Noll (1965), and Naghdi (1972, 1982). It should be remarked, however, that due to the differences in physical structure of the phenomena considered, the development of the dynamical theory with the use of a triad of directors in this paper is substantially different than those formulated in previous works. Despite this, mention may be made of a striking mathematical similarity between the basic dynamical equations (in direct notation) for shell-like bodies given in Naghdi (1982, §8) and those developed in §4 of the present paper.

(a) *A summary description of the major results obtained*

A general idea of the scope of the paper can be had from a list of contents preceding the abstract. Here we highlight some of the main results. After presenting in §2 a brief overview of microscopic and submicroscopic features of a crystal lattice in the context of inelastic behaviour, a triad of directors is introduced to represent the effect of lattice vectors at the macroscopic scale. Kinematics of the lattice structure in the macroscopic theory, based on continuous distributions of dislocations, are discussed in some detail in §3 and include:

1. The identification of a measure of plastic deformation tensor G_p (see (3.8)) which is the composition of the inverse of the lattice deformation tensor $_\ell F$ and the deformation gradient F. This identification is accomplished by using the notion of a mechanically reversible motion associated with an intermediate configuration which is defined (locally) in terms of G_p. This manner of introducing an intermediate configuration is in contrast to a procedure adopted during the past 25 years in some of the literature on plasticity, where a multiplicative decomposition of F is used after first defining a 'stress-free' intermediate configuration; in this connection, see §4 of the review article by Naghdi (1990).

2. The stretch and rotation associated with the lattice deformation tensor $_\ell F$ and the plastic deformation tensor G_p, as well as a derived equation relating G_p to the plastic strain E_p (see (3.27)).

3. A kinematical development resulting in the relationship between the gradient of G_p, the Burgers vector and the dislocation density per unit area in the reference configuration. This development differs from those of Eshelby (1956) and Bilby (1960) who have defined the dislocation density in terms of elastic lattice deformations, while the present development with the use of the gradient of G_p provides a connection between changes in dislocation density to processes involving plastic deformation. In this connection, it should be noted that while *formal* compositions similar to the tensor G_p and its relationship to the dislocation density have been proposed in a number of papers beginning with Bilby *et al.* (1957), the identification of the tensor G_p in the present paper involves the notion of mechanical reversibility and is complete only after it is shown (with the use of the balance laws and constitutive equations in §§4–6) that processes in which the rate of $G_p \neq 0$ are irreversible.

Some of the main results in the remainder of the paper (§§4–6), which are concerned with the balance laws and the construction of general constitutive equations for structured solids, are:

4. The statement of the additional momentum-like balance laws (see (4.11)) which include the effect of inertia associated with plastic deformation. This effect plays a significant role in the subsequent development of the dynamical theory for both viscoplasticity and (the more usual) rate-independent plasticity.

5. Development of a general constrained theory for materials possessing an elastic range and the manner that the constraint gives rise to a yield function Φ (see (5.9)). This function delineates the elastic range; and, in turn, leads to the introduction of yield function g in the space of the basic kinematical variables corresponding to Φ.

6. An expression for the rate of energy dissipation ξ (see (6.13)) – derived in the context of the constrained theory – involves two of the main constitutive response functions, one of which is the constitutive tensor response function $\hat{K}$ representing the effect of the intrinsic director force (or the intrinsic lattice force) per unit volume in the reference configuration.

7. Subsequent use of the expression for the rate of energy dissipation allows (without any additional assumption) to express the constitutive response function $\hat{K}$ as a linear sum of three response functions in (6.16), namely $\hat{K}_1$, $\hat{K}_2$ and $\hat{K}_3$. The first of these, i.e. the tensor function $\hat{K}_1$, depends only on the kinematical variables $\mathcal{U}$ defined by $(5.6)_1$ and is entirely independent of rate quantities; the second, i.e. $\hat{K}_2$, depends on $\mathcal{U}$ and a unit tensor representing the direction ρ of the rate of plastic deformation; and the third, i.e. $\hat{K}_3$, depends on $\mathcal{U}$, as well as both the unit tensor ρ and the magnitude γ of the rate of plastic deformation.

8. A geometrical interpretation of the response function $\hat{K}_2$ leading to the result that the values of $\hat{K}_2$ lie on a hypersurface represented by Φ_2 (see (6.23)). The surface Φ_2 is referred to as the loading surface since the response function $\hat{K}_2$ must always lie on this surface during processes that give rise to plastic deformations.

9. The identification of the response function $\hat{K}_3$ as a viscoplastic response; and $\hat{K}_2$, which when inverted, results in an equation analogous to the constitutive equation for the plastic strain rate in the usual formulation of elastic-plastic behaviour.

10. A discussion of the continuity conditions leading to the effect that the two hypersurfaces Φ and Φ_2 become coincident if either $\overset{\circ}{K}$ in (6.17) is a continuous function of time or if the inertia term in the balance equation $(4.13)_1$ vanishes.

(b) *Notation and mathematical preliminaries*

We close this section with a short glossary of notations and some mathematical terminology. Any linear mapping from V, the three-dimensional translation vector space associated with the euclidean point space $\mathscr{E}$, into V will be called a second-order tensor. The trace and determinant functions of second-order tensors will be denoted, respectively, by tr and det. The transpose of the second-order tensor T will be denoted by T^{T}, its inverse if it exists by T^{-1} and the inverse of its transpose (i.e. $(G_{\mathrm{p}}^{-1})^{\mathrm{T}}$) by $G_{\mathrm{p}}^{-\mathrm{T}}$. The usual inner product on V is written as $a \cdot b$ for any two vectors $a, b \in V$ and the (induced) norm, or magnitude, of a is given by $\|a\| = (a \cdot a)^{\frac{1}{2}}$. An inner product for second-order tensors A, B is defined by $A \cdot B = \mathrm{tr}(A^{\mathrm{T}}B)$ with the associated norm $\|A\| = (A \cdot A)^{\frac{1}{2}}$. The tensor product $a \otimes b$ of any two vectors $a, b \in V$ is the second-order tensor defined by $(a \otimes b)v = (b \cdot v)a$ for every vector v and the identity tensor is denoted by I. Generally, direct tensor notation is used in the paper and summation over repeated subscript and superscript is understood as, for example, in $(3.6)_{1,2}$. The notations 'grad' and 'div' stand, respectively, for the gradient and divergence operators with respect to reference position X. Also, a

superposed dot signifies material time differentiation and a comma following a subscript indicates partial differentiation. We denote the basis vectors in the reference and the current configurations by $\{E_A\}$ and $\{e_i\}$, respectively, where both subscripts have the range $A = 1, 2, 3$ and $i = 1, 2, 3$. Occasionally, we find it convenient to record components of various expressions with respect to a fixed orthonormal basis $\{E_A\}$ for vectors and tensor fields defined on the reference configuration, or to speak of components of tensor fields such as δ_{AB} of I referred to the basis $E_A \otimes E_B$ and F_{iA} (or $x_{i,A}$) referred to basis $e_i \otimes E_A$.

A notation of the type $\mathscr{L}[b]$ signifies operation of a linear operator $\mathscr{L}$ such as a second-order (fourth-order) tensor acting on a first-order (second-order) tensor. Thus, if $A = A_{KL} E_K \otimes E_L$ is a second-order tensor and if $b = b_K E_K$ is a vector, we write $A[b]$ to mean $(A_{KL} b_L) E_K$. Similarly, if $C = C_{KLMN} E_K \otimes E_L \otimes E_M \otimes E_N$ is a fourth order tensor, we write $C[A]$ to mean $C_{KLMN} A_{MN} E_K \otimes E_L$.

Finally, a comment may be made about the notation for certain fields which occur in the referential (lagrangian) formulation of the dynamical equations of §4. A subscript R is attached to certain symbols (such as $_R k^A$, $_R m^A$ and $_R K$, $_R M$ in $(4.1)_{2,3}$) that define kinetical entities over the reference configuration to avoid confusion with the fairly standard use of the same symbols without the subscript R in a corresponding spatial (eulerian) formulation of a Cosserat continuum.

2. Background remarks on microscopic and submicroscopic descriptions of the crystal lattice and dislocations

The macroscopic theory of the inelastic behaviour of crystals constructed in §§3 and 4 and utilized in the remainder of the paper uses three additional (independent) kinematical variables denoted by d_A ($A = 1, 2, 3$), which characterize certain features of the crystal lattice structure on the microscopic and submicroscopic levels. As will become clear in the subsequent sections, explicit identification of these macroscopic variables with appropriate microscopic and submicroscopic features is essential for motivating the forms of the constitutive equations of the macroscopic responses of the medium, as well as for physically meaningful interpretation of the macroscopic results. Preparatory to this objective and for the sake of clarity, we focus here on some background remarks pertinent to inelastic deformation of a single crystal in terms of the microscopic and submicroscopic descriptions of the material.

When a single crystal undergoes a motion which results in a permanent deformation (on the macroscopic scale) such as elastic-plastic or elastic-viscoplastic, several microstructural features of the motion can be seen with increasing detail at various progressively finer scales of motion. Thus, while the crystal appears quite smooth on the macroscale, the deformation is seen to be composed of many closely spaced steps at a magnification of about $150 \times$ (see Guinier & Jullien 1989, p. 193, fig. 4.12). As the magnification is increased further to about $35000 \times$, first slip bands and then dislocation clusters begin to appear (see Guinier 1984, p. 113, fig. 5.10). Even at this scale the atomic lattice is not visible, even though it may be inferred from other observations. The cores of dislocations and the lattice distortions can be seen at levels of about $10^6 \times$ magnification (see Guinier 1984, p. 122, fig. 5.9).

It should be emphasized that the aim of the present paper is the development of a (macroscopic) theory based on a continuous distribution of dislocations which can be observed in the range of magnification of roughly approaching $10^5 \times$, and thus

ignore a more detailed feature of the material behaviour such as the exact arrangement of the core of dislocation observed only at approximately $10^6 \times$ magnification. Hence, in the present context, any description of material behaviour at a scale approaching the atomic level serves only as a 'background' model for the (macroscopic) continuum theory. By this we mean that while certain features of the dislocation motion at the submicroscopic level can be represented effectively in the macroscopic theory, one is not interested in every detail of the randomly distributed dislocation motion at the atomic level, i.e. one is not interested in the location of every atom for all times.

(a) Crystal deformations at the microscopic and submicroscopic scales

It is convenient at this point to introduce some notations pertaining to the microscopic description of the body. A fixed reference configuration κ_0^* of the body $\mathscr{B}$ bounded by $\partial \mathscr{B}$ occupies a region $\mathscr{R}_0^*$ bounded by a closed surface $\partial \mathscr{R}_0^*$; and in the configuration κ^* at time t, the body occupies a region $\mathscr{R}^*$ bounded by a closed surface $\partial \mathscr{R}^*$. (The use of the asterisk attached to the various symbols is for later convenience. The corresponding symbols without the asterisk are reserved for different designations to be introduced in §3.) Any arbitrary material volume $\mathscr{S}^*$ of $\mathscr{B}$ in the two configurations κ_0^* and κ^* occupy, respectively, the regions $\mathscr{P}_0^*$ ($\subseteq \mathscr{R}_0^*$) bounded by the closed surface $\partial \mathscr{P}_0^*$ and $\mathscr{P}^*$ ($\subseteq \mathscr{R}^*$) bounded by a closed surface $\partial \mathscr{P}^*$. Any microscopic material point (or particle) X^* within $\mathscr{S}^*$ in the configurations κ^* and κ_0^* is identified by the position vectors x^* and X^*, respectively. We further designate the location of the centre of mass of $\mathscr{S}^*$ in the current and reference configurations by x and X, respectively. The adoption of these designations here are in anticipation of later identification of centre of mass of $\mathscr{S}^*$ in κ^* and κ_0^* (in §3) with the position vectors x and X of a material point in the macroscopic theory. (This, of course, means that the entire part $\mathscr{S}^*$ (on the microscopic scale) is associated with a single material point (or particle) X on the macroscopic scale.)

We represent the periodic arrangement of the crystal lattice at each particle X^* of $\mathscr{S}^*$ by means of vectors d_A^* and D_A^* ($A = 1, 2, 3$) in the configurations κ^* and κ_0^*, respectively. We refer to these vectors as *lattice vectors* and stipulate further that the lattice vectors are non-coplanar at all times. Next, we introduce the vectors d_A and D_A through the formulae

$$d_A = \frac{1}{V^*} \int_{\mathscr{P}^*} d_A^* \, dv, \quad D_A = \frac{1}{V_0^*} \int_{\mathscr{P}_0^*} D_A^* \, dV \quad (A = 1, 2, 3), \tag{2.1}$$

where V^* and V_0^* are the volumes of $\mathscr{S}^*$ in the current and reference configurations, respectively. The vectors d_A and D_A in (2.1), which represent the averaged or 'smeared' lattice structure of the crystal, are in general different from the lattice vectors and will be referred to as the *lattice directors*. Further, the sets of vectors $\{d_1, d_2, d_3\}$ and $\{D_1, D_2, D_3\}$ are each assumed to be non-coplanar. This implies that the scalar triple product for each set is non-zero, i.e.

$$[d_1 \, d_2 \, d_3] \neq 0, \tag{2.2}$$

with a similar condition holding for the vectors D_A ($A = 1, 2, 3$). This permits us to define the reciprocal vectors (or dual vectors) d^A and D^A, through the relations

$$d^B \cdot d_A = D^B \cdot D_A = \delta_A^B, \tag{2.3}$$

where the symbol δ_A^B stands for the Kronecker delta. The lattice vectors (and hence the lattice directors) have the physical dimensions of length so that the dual vectors $\boldsymbol{d}^B$ and $\boldsymbol{D}^B$ have the physical dimensions of 1/length.

3. Kinematics of the lattice structure in the macroscopic theory

In the usual macroscopic description of materials, a body $\mathscr{B}$ bounded by a surface $\partial\mathscr{B}$ is regarded as consisting of a set of material points (or particles) X. Here, in the context of directed media, let each material point X be endowed with additional kinematical variables represented by a triad of independent vector fields called *directors*. Remembering the background information at the microscopic scale indicated in §2, the directors may be regarded as representing an equivalent lattice structure of the crystal on the macroscopic scale. Thus, in a fixed reference configuration $\boldsymbol{\kappa_0}$ of $\mathscr{B}$, let the material point X and the directors at X be identified, respectively, by the position vector $\boldsymbol{X}$ and the values of the director triads $\boldsymbol{D}_A = \boldsymbol{D}_A(X)$ $(A = 1, 2, 3)$; and, similarly, denote the corresponding quantities in the current configuration $\boldsymbol{\kappa}$ at time t by the position vector $\boldsymbol{x}$ and the director triads $\boldsymbol{d}_A$ at $\boldsymbol{x}$ $(A = 1, 2, 3)$. (It is understood that the symbols such as $\boldsymbol{\kappa_0}$, $\boldsymbol{\kappa}$ (without an asterisk) in this section are associated with configurations in the macroscopic description of the motion of $\mathscr{B}$.) We define a set of two sufficiently smooth vector functions $\boldsymbol{\chi}$ and $\mathscr{D}_A$ $(A = 1, 2, 3)$, which respectively assign the place $\boldsymbol{x}$ and the director triads $\boldsymbol{d}_A$ to each material point in the current configuration $\boldsymbol{\kappa}$ of $\mathscr{B}$ at time t, i.e.

$$\boldsymbol{x} = \boldsymbol{\chi}(X, t), \quad \boldsymbol{d}_A = \bar{\mathscr{D}}_A(\boldsymbol{D}_B, t; X) = \mathscr{D}_A(X, t) \quad (A, B = 1, 2, 3). \tag{3.1}$$

The functional form of $\bar{\mathscr{D}}_A$ in the first of $(3.1)_2$ is intended to emphasize its explicit dependence on X. The set of two functions $\{\boldsymbol{\chi}, \mathscr{D}_A\}$ will be referred to as a *process*. (By a process we mean that the functions $\boldsymbol{\chi}$ and $\mathscr{D}_A$ must be determined from relevant balance laws and must be also compatible with appropriate constitutive equations.) The function $\boldsymbol{\chi}$ is called a motion and an explicit physically relevant identification of the vector functions $\mathscr{D}_A$ will be made presently. We assume that the triad of directors is non-coplanar so that we may introduce the reciprocal director triads $\boldsymbol{D}^A$ and $\boldsymbol{d}^A$ satisfying the relations (2.3). The deformation gradient $\boldsymbol{F}$ and its determinant are defined by

$$\boldsymbol{F} = \partial\boldsymbol{\chi}/\partial\boldsymbol{X}, \quad J = \det\boldsymbol{F}. \tag{3.2}$$

We assume that $(3.1)_1$, but not $(3.1)_2$, is invertible for a fixed value of t so that the jacobian of transformation associated with $(3.1)_1$ does not vanish; and for definiteness, we further stipulate that $J > 0$.

The ordinary particle velocity $\boldsymbol{v}$ and director velocities $\boldsymbol{w}_A$ are defined by

$$\boldsymbol{v} = \dot{\boldsymbol{x}}, \quad \boldsymbol{w}_A = \dot{\boldsymbol{d}}_A \quad (A = 1, 2, 3), \tag{3.3}$$

where a superposed dot denotes material time differentiation with respect to t holding $\boldsymbol{X}$ fixed.

We also recall the well-known expression that relates a line element $\mathrm{d}\boldsymbol{x}$ in the current configuration $\boldsymbol{\kappa}$ to its image $\mathrm{d}\boldsymbol{X}$ in the fixed reference configuration $\boldsymbol{\kappa_0}$ and similarly that which relates the time derivative of $\mathrm{d}\boldsymbol{x}$ in $\boldsymbol{\kappa}$ to its image in $\boldsymbol{\kappa_0}$, i.e.

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{F}\mathrm{d}\boldsymbol{X}, \quad \overline{\dot{\mathrm{d}\boldsymbol{x}}} = \boldsymbol{L}\,\mathrm{d}\boldsymbol{x} = \dot{\boldsymbol{F}}\mathrm{d}\boldsymbol{X}, \tag{3.4}$$

where

$$\dot{\boldsymbol{F}} = \boldsymbol{L}\boldsymbol{F}, \quad \boldsymbol{L} = \partial\boldsymbol{v}/\partial\boldsymbol{x}. \tag{3.5}$$

(a) *Identification of a measure of plastic deformation*

Recalling the background discussion in §2 concerning the lattice vectors and the lattice directors, we now proceed to introduce a (dimensionless) two-point tensor field denoted by $_\ell F$ and called the *lattice deformation tensor* which is defined as the tensor product of the lattice directors in κ defined by $(2.1)_1$ with their duals in κ_0 defined by $(2.1)_2$. This lattice deformation tensor $_\ell F$, its inverse and its determinant are given by the formulae

$$_\ell F = d_A \otimes D^A, \quad _\ell F^{-1} = D_A \otimes d^A, \quad _\ell J = \det[_\ell F] \neq 0, \tag{3.6}$$

and note that from (3.6) follow the expressions

$$\left. \begin{aligned} d_A &= {_\ell F} D_A, \quad D_A = {_\ell F^{-1}} d_A, \\ d^A &= ({_\ell F^{-1}})^{\mathrm{T}} D^A, \quad D^A = {_\ell F^{\mathrm{T}}} d^A \quad (A = 1, 2, 3), \end{aligned} \right\} \tag{3.7}$$

where summation over the repeated subscript and superscript A in (3.6) is understood. It should be clear that the role of the lattice deformation tensor $_\ell F$ between the director triads d_A and D_A in (3.7) is akin to that of the deformation gradient F between dx and dX in $(3.4)_1$. Moreover, it is important to note that while $(3.4)_1$ is integrable, $(3.7)_1$ is not; the latter, of course, implies that $_\ell F$ is not integrable.

Before the identification of a measure of plastic (or inelastic) deformation, for clarity's sake, we need to dispose of some additional preliminaries. Thus, as indicated earlier, we identify the position x with the centre of mass of a microscopic material region and the vector triad d_A with a mean lattice structure located at x (see equations (2.1)). Further, we recall that the usual elasticity theory is considered to be reversible in the sense that, following any motion or deformation from a reference state, the material can always be returned to its reference state simply by reversing the motion; the reference state may, of course, be taken as the initial state. Recalling the notion of a process introduced following (3.1), we now consider a special process in which the lattice directors behave as material line elements. It then follows that for such a process the vector functions $\mathscr{D}_A$ are determined by the motion χ. Further, the lattice directors along with all the macroscopic particles in the body may be returned to their reference state simply by reversing the motion χ of the body. Consider now a special cycle consisting of the special process and its reverse. We assume that for all such cycles during which the lattice directors behave as material line elements, the external work done on the body is zero. It then follows that all such processes are mechanically reversible. (A full discussion of such mechanically reversible processes requires consideration of the complete dynamical theory, including the constitutive equations. For this reason we postpone further remarks on this point until §6.)

Any arbitrary process of the crystal is not necessarily reversible on the microscopic or submicroscopic scale. This is because the relative positions of the microscopic particles may be altered by inelastic processes and hence the lattice structure does not return to its original state upon reversal of the macroscopic deformation. To elaborate, consider a typical process which, on the macroscopic scale, takes a material point (or particle) to its corresponding point x in the current configuration κ of the body at time t. Such a process is not necessarily reversible. However, it is possible to associate with a given arbitrary process a reversible process resulting in the same place x in κ such that the lattice directors behave as material line elements and the tensor $_\ell F$ in (3.7) is the same as the deformation gradient F. Clearly the

lengths and orientations of the lattice directors at the same material point will be different for irreversible and reversible processes. This suggests that the difference between the functions $\boldsymbol{F}$ and $_{\ell}\boldsymbol{F}$ may be used as a measure of permanent deformation in a crystal and leads us to introduce a tensor $\boldsymbol{G}_{\mathrm{p}}$ through the relation

$$\boldsymbol{G}_{\mathrm{p}} = {}_{\ell}\boldsymbol{F}^{-1}\boldsymbol{F}. \tag{3.8}$$

In what follows, the tensor $\boldsymbol{G}_{\mathrm{p}}$ will be referred to as the plastic deformation in anticipation of its identification (or prescription) based on certain results to be established in §6, where it is shown that the processes for which $\dot{\boldsymbol{G}}_{\mathrm{p}} \neq 0$ are dissipative and hence irreversible.

It may be emphasized that in defining (3.8) we have appealed to the notion of a reversible process discussed in the penultimate paragraph. This definition of $\boldsymbol{G}_{\mathrm{p}}$ can now be utilized to define a unique 'local' intermediate configuration. But before embarking on this, for clarity's sake it is important to indicate that the term 'local' is used here to mean an infinitesimal neighbourhood, i.e. the tangent space at a given material point of the body manifold. (This usage of the term 'local', which is common throughout the literature in continuum mechanics, is in contrast to the modern usage of the same word in mathematics where the term 'local' is used to mean a finite (not necessarily small) neighbourhood of a point.) Keeping this background in mind, we now define a unique local intermediate configuration by means of the following procedure: From the present configuration $\boldsymbol{\kappa}$, we map the body into an intermediate configuration $\bar{\boldsymbol{\kappa}}$ by means of a local process such that at every material point (1) the lattice directors behave as material line elements, and (2) the lattice directors $\bar{\boldsymbol{d}}_A$ in $\bar{\boldsymbol{\kappa}}$ coincide with the lattice directors $\boldsymbol{D}_A$ in the reference configuration $\boldsymbol{\kappa}_0$.

Such a configuration can be achieved locally for every material point by means of a deformation tensor $_{\ell}\boldsymbol{F}^{-1}$ with respect to the present configuration and we may write

$$\mathrm{d}\bar{\boldsymbol{x}} = {}_{\ell}\boldsymbol{F}^{-1}\mathrm{d}\boldsymbol{x}, \quad \bar{\boldsymbol{d}}_A = {}_{\ell}\boldsymbol{F}^{-1}\boldsymbol{d}_A, \tag{3.9}$$

both of which are linear transformations taking a line element $\mathrm{d}\boldsymbol{x}$ into $\mathrm{d}\bar{\boldsymbol{x}}$ and the lattice directors $\boldsymbol{d}_A$ into $\bar{\boldsymbol{d}}_A$. (It should be clear that in the context of the present paper $(3.9)_1$ must be viewed as a relation between the infinitesimal displacements $\mathrm{d}\boldsymbol{x}$ and $\mathrm{d}\bar{\boldsymbol{x}}$, i.e. tangent vectors at the material point $\boldsymbol{x}$.) Since both $\mathrm{d}\boldsymbol{x}$ and $\boldsymbol{d}_A$ in (3.9) transform by $_{\ell}\boldsymbol{F}^{-1}$, the requirement (1) is satisfied. Substitution of $(3.7)_2$ into $(3.9)_2$, at once yields

$$\bar{\boldsymbol{d}}_A = \boldsymbol{D}_A, \tag{3.10}$$

which meets the requirement (2). This demonstrates the existence of a configuration $\bar{\boldsymbol{\kappa}}$ as defined by (1) and (2) above. To show uniqueness, suppose that there exists another configuration $\hat{\boldsymbol{\kappa}}$ satisfying (1) and (2) such that $\mathrm{d}\hat{\boldsymbol{x}} \neq {}_{\ell}\boldsymbol{F}^{-1}\mathrm{d}\boldsymbol{x}$ and by (1) $\hat{\boldsymbol{d}}_A \neq {}_{\ell}\boldsymbol{F}^{-1}\boldsymbol{d}_A$. The latter by $(3.7)_2$ implies that $\hat{\boldsymbol{d}}_A \neq \boldsymbol{D}_A$ which contradicts the requirement (2). This establishes the uniqueness of the procedure for identification of the intermediate configuration $\bar{\boldsymbol{\kappa}}$. (The procedure for the identification of $\bar{\boldsymbol{\kappa}}$ described here should not be confused with any multiplicative decomposition associated with an intermediate stress free configuration introduced in the context of macroscopic theories of plasticity by other authors. Setting aside the matter of uniqueness for any such configuration, it may be noted that $\bar{\boldsymbol{\kappa}}$ as defined by the requirements (1) and (2) is not necessarily stress free and therefore will be free from any physical difficulties associated with its existence.) Substituting for the vectors $\mathrm{d}\boldsymbol{x}$ and $\boldsymbol{d}_A$ in the above equations (3.9) and (3.10) by means of the relations $(3.4)_1$ and $(3.7)_1$, respectively, we

arrive at the following representations for the line element $\mathrm{d}\bar{x}$ in terms of the reference line element $\mathrm{d}X$:

$$\mathrm{d}\bar{x} = G_{\mathrm{p}}\,\mathrm{d}X. \tag{3.11}$$

A schematic diagram of the reference, intermediate and current configurations is shown in figure 1. During the deformation from the configuration κ_0 to $\bar{\kappa}$, G_{p} acts on the material line element $\mathrm{d}X$ but not on the vectors D_A representing the lattice structure. It is important to note that $\bar{\kappa}$ is a collection of tangent spaces, i.e. a collection of local configurations which do not continuously fit together to form a global configuration. This is due to the fact that G_{p} need not satisfy any integrability condition, and consequently no position vector can be assigned to $\bar{\kappa}$.

It can be seen that the tensor G_{p} introduced above has the following properties: (i) in the reference configuration $_\ell F = F = I$, and hence $G_{\mathrm{p}} = I$; (ii) during a purely elastic deformation from a reference state, the lattice directors behave as line elements of ordinary continuum so that $_\ell F = F$ and $G_{\mathrm{p}} = I$ and hence the intermediate configuration $\bar{\kappa}$ coincides with κ_0; and (iii) it can also be shown that if further deformation from any configuration is purely elastic, then $\dot{G}_{\mathrm{p}}$ vanishes (see (3.14) below).

We continue our discussion of kinematics and proceed to establish an additional result which justifies the choice (3.8) as a measure of plastic deformation. To this end, taking the material time derivative of (3.8) we obtain

$$\dot{G}_{\mathrm{p}} = {}_\ell F^{-1}\dot{F} + \overline{{}_\ell\dot{F^{-1}}}F = {}_\ell F^{-1}(L - {}_\ell\dot{F}\,{}_\ell F^{-1})F. \tag{3.12}$$

In writing $(3.12)_2$ use has been made of $(3.5)_1$, as well as ${}_\ell F^{-1}{}_\ell F = I$ and its time derivative, where I denotes the identity tensor. According to (B 6) of Appendix B, during elastic processes only the rate of lattice deformation tensor $_\ell\dot{F}$ can be related to $_\ell F$ by a formula analogous to $(3.5)_1$, namely

$$_\ell\dot{F} = L\,{}_\ell F \quad \text{for reversible processes.} \tag{3.13}$$

Substitution of (3.13) into $(3.12)_2$ easily reveals that the quantity in parentheses on the right-hand side of $(3.12)_2$ vanishes and hence

$$\dot{G}_{\mathrm{p}} = 0 \quad \text{for reversible processes.} \tag{3.14}$$

Now for any function ϕ (not necessarily a scalar) of the variables $(F, {}_\ell F)$, if adopted as a measure of plastic deformation, the values of the function must remain unchanged during elastic processes and hence must satisfy the condition

$$\dot{\phi} = 0 \quad \text{for reversible processes.} \tag{3.15}$$

We now prove the following:

Theorem 3.1. *Let ϕ be any function of the variables $(F, {}_\ell F)$ that satisfies the condition* (3.15) *during elastic processes. Then, since G_{p} also satisfies* (3.15) *by virtue of* (3.14), *it is both necessary and sufficient that ϕ must have the form*

$$\phi = \bar{\phi}(G_{\mathrm{p}}). \tag{3.16}$$

The proof of sufficiency is trivial. Indeed, if ϕ has the form (3.16), then $\dot{\phi} = (\partial\bar{\phi}/\partial G_{\mathrm{p}})\cdot\dot{G}_{\mathrm{p}}$ and by virtue of (3.14) the conditions (3.15) is satisfied. To prove necessity, we observe that any function $\hat{\phi}(F, {}_\ell F)$ with the help of (3.8) can be expressed as a different function of $(G_{\mathrm{p}}, {}_\ell F)$, i.e.

$$\phi = \hat{\phi}(F, {}_\ell F) = \hat{\phi}({}_\ell F\,G_{\mathrm{p}}, {}_\ell F) = \bar{\phi}(G_{\mathrm{p}}, {}_\ell F). \tag{3.17}$$

Taking the material time derivative of $(3.17)_3$, we obtain

$$\dot{\phi} = \frac{\partial \overline{\phi}}{\partial \boldsymbol{G}_{\mathrm{p}}} \cdot \dot{\boldsymbol{G}}_{\mathrm{p}} + \frac{\partial \overline{\phi}}{\partial \,_{\ell}\boldsymbol{F}} \cdot \,_{\ell}\dot{\boldsymbol{F}}. \tag{3.18}$$

In view of (3.14) and (3.13), during elastic processes (3.18) becomes

$$\dot{\phi} = \frac{\partial \overline{\phi}}{\partial \,_{\ell}\boldsymbol{F}} (\boldsymbol{L} \,_{\ell}\boldsymbol{F}) = 0. \tag{3.19}$$

The last result must hold for all non-zero values of $(\boldsymbol{L}, \,_{\ell}\boldsymbol{F})$; and, moreover, on account of continuity must also hold for all processes. Hence $\partial \overline{\phi}/\partial \,_{\ell}\boldsymbol{F} = \boldsymbol{0}$ and this, in turn, implies that ϕ must be of the form (3.16) and the proof is complete.

From the above theorem, we conclude that every choice of ϕ as a measure of plastic deformation must have the form (3.16); and, hence, without ambiguity we may choose $\boldsymbol{G}_{\mathrm{p}}$ itself as a measure of plastic deformation as proposed earlier by (3.8).

Since by $(\mathrm{B}\,6)_2$ of Appendix B the expression $\dot{\boldsymbol{d}}_A = \boldsymbol{L}\boldsymbol{d}_A$ holds for elastic processes only, the difference vector $(\dot{\boldsymbol{d}}_A - \boldsymbol{L}\boldsymbol{d}_A)$ at a given instant of time represents the rate of change of the lattice directors in excess of the rate of change of material line elements which coincide with them at that instant. With the help of $(3.7)_1$, the above difference vector can be expressed as

$$\dot{\boldsymbol{d}}_A - \boldsymbol{L}\boldsymbol{d}_A = (\,_{\ell}\dot{\boldsymbol{F}} - \boldsymbol{L} \,_{\ell}\boldsymbol{F}) \boldsymbol{D}_A. \tag{3.20}$$

Premultiplying (3.12) with $\,_{\ell}\boldsymbol{F}$ and postmultiplying with $\boldsymbol{G}_{\mathrm{p}}^{-1}$ and after using (3.8), we obtain an expression which is equal to the negative of the right-hand side of (3.20). Then by comparing the latter expression with (3.20) we arrive at

$$\dot{\boldsymbol{d}}_A - \boldsymbol{L}\boldsymbol{d}_A = -(\,_{\ell}\boldsymbol{F}\dot{\boldsymbol{G}}_{\mathrm{p}} \boldsymbol{G}_{\mathrm{p}}^{-1}) \boldsymbol{D}_A. \tag{3.21}$$

The above expression for the difference vector $(\dot{\boldsymbol{d}}_A - \boldsymbol{L}\boldsymbol{d}_A)$ plays an important role in statement of one of the balance laws in §4.

(b) *The stretch and rotation associated with the lattice deformation tensor $\,_{\ell}\boldsymbol{F}$ and the plastic deformation tensor $\boldsymbol{G}_{\mathrm{p}}$*

We discuss here the local stretch and rotation associated with the second order tensors $\,_{\ell}\boldsymbol{F}, \boldsymbol{G}_{\mathrm{p}}$ and consider their relationships to the stretch and rotation associated with the deformation gradient $\boldsymbol{F}$. According to the polar decomposition theorem (see Truesdell & Noll 1965), any non-singular (invertible) second order tensor $\boldsymbol{Z}$ can be uniquely decomposed in the form

$$\boldsymbol{Z} = \boldsymbol{R}\boldsymbol{U} = \boldsymbol{V}\boldsymbol{R}, \tag{3.22}$$

where $\boldsymbol{R}$ is a proper orthogonal tensor and both $\boldsymbol{U}$ and $\boldsymbol{V}$ are symmetric positive definite second-order tensors.

In what follows immediately, we consider only $(3.22)_1$ and postpone the use of $(3.22)_2$ until later in this subsection. Thus, applying $(3.22)_1$ to each of the three tensors $\boldsymbol{F}, \,_{\ell}\boldsymbol{F}$ and $\boldsymbol{G}_{\mathrm{p}}$, we have

$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U}, \quad \,_{\ell}\boldsymbol{F} = \,_{\ell}\boldsymbol{R} \,_{\ell}\boldsymbol{U}, \quad \boldsymbol{G}_{\mathrm{p}} = \boldsymbol{R}_{\mathrm{p}} \boldsymbol{U}_{\mathrm{p}}, \tag{3.23}$$

where the tensors $\boldsymbol{R}, \,_{\ell}\boldsymbol{R}$ and $\boldsymbol{R}_{\mathrm{p}}$ each satisfy conditions of the type

$$\boldsymbol{R}\boldsymbol{R}^{\mathrm{T}} = \boldsymbol{R}^{\mathrm{T}}\boldsymbol{R} = \boldsymbol{I}, \quad \det \boldsymbol{R} = 1, \tag{3.24}$$

while $\boldsymbol{U}, \,_{\ell}\boldsymbol{U}$ and $\boldsymbol{U}_{\mathrm{p}}$ are given by

$$\boldsymbol{U}^2 = \boldsymbol{F}^{\mathrm{T}}\boldsymbol{F} = \boldsymbol{C}, \quad \,_{\ell}\boldsymbol{U}^2 = \,_{\ell}\boldsymbol{F}^{\mathrm{T}} \,_{\ell}\boldsymbol{F} = \,_{\ell}\boldsymbol{C}, \quad \boldsymbol{U}_{\mathrm{p}}^2 = \boldsymbol{G}_{\mathrm{p}}^{\mathrm{T}} \boldsymbol{G}_{\mathrm{p}} = \boldsymbol{C}_{\mathrm{p}}. \tag{3.25}$$

The second-order tensor C in the first of (3.25) is the familiar right Cauchy–Green measure of deformation and in the second and third of (3.25) we have introduced analogous measures for lattice deformation tensor $_\ell C$ and C_p associated with plastic deformation G_p. It is convenient at this point to recall the familiar lagrangian measure of relative strain E and also for later use to introduce analogous expressions for the lagrangian lattice strain $_\ell E$ and the plastic strain E_p. These are defined by

$$E = \tfrac{1}{2}(C-I), \quad _\ell E = \tfrac{1}{2}(_\ell C - I), \quad E_p = \tfrac{1}{2}(C_p - I). \tag{3.26}$$

Moreover, since $_\ell F = FG^{-1}$ by (3.8), $(3.26)_2$ can be expressed as

$$_\ell E = \tfrac{1}{2}\{(FG_p^{-1})^\mathrm{T}\,(FG_p^{-1}) - I\}.$$

After using the indicated transposition, substituting $G_p^{-\mathrm{T}}\,G_p^\mathrm{T}\,G_p\,G_p^{-1}$ for the identity tensor and invoking $(3.25)_3$, the last expression can be reduced to

$$_\ell E = G_p^{-\mathrm{T}}(E - E_p)\,G_p^{-1}, \tag{3.27}$$

where in obtaining (3.27) use has also been made of $(3.26)_{1,3}$.

To examine locally the nature of deformation resulting from a process specified by $(3.1)_{1,2}$ and to assign suitable interpretations to the various tensorial quantities in (3.23)–(3.25), we need to consider the action of these tensors on material line elements and lattice directors at a given material point. Remembering the notations for the material line elements in configurations κ_0 and κ and since the body (here a crystal) is embedded in a three-dimensional euclidean space, it will suffice to consider the deformation of three mutually orthogonal line elements dX_A, namely

$$dx_A = F\,dX_A, \quad d\bar{x}_A = G_p\,dX_A \quad (A = 1,2,3). \tag{3.28}$$

Let the magnitudes of dX_A, dx_A and $d\bar{x}_A$ be denoted by dS_A, ds_A and $d\bar{s}_A$, respectively, and introduce the unit vectors M_A in the direction of dX_A, m_A in the direction of dx_A and $\bar{m}_A$ in the direction of $d\bar{x}_A$. The three unit vectors M_A, without loss in generality, may be identified with orthonormal basis E_A in κ_0. In general, the line elements dX_A undergo both stretch and rotation and the ratios $(ds_1/sS_1, ds_2/dS_2, ds_3/dS_3)$ denoted by λ_A $(A = 1,2,3)$ are called the stretch of the line elements. Corresponding stretches in the intermediate configuration $\bar{\kappa}$ (see figure 1) may be defined analogously. These observations may be summarized as follows:

$$\left.\begin{aligned}
&dX_A = E_A\,dS_A, \quad dx_A = m_A\,ds_A, \quad d\bar{x}_A = \bar{m}_A\,d\bar{s}_A \quad (\text{no sum on } A),\\
&\lambda_A^2 = ds_A^2/dS_A^2 = M_A\cdot CM_A, \quad \bar{\lambda}_A^2 = ds_A^2/d\bar{s}_A^2 = \bar{M}_A\cdot{}_\ell C\bar{M}_A \quad (\text{no sum on } A),\\
&(\lambda_A^p)^2 = d\bar{s}_A^2/dS_A^2 = M_A\cdot(C_p[M_A]) \quad (\text{no sum on } A).
\end{aligned}\right\} \tag{3.29}$$

Similarly, let the magnitudes of D_A, d_A and $\bar{d}_A = D_A$ (see (3.10)) be denoted by D_A, d_A and $\bar{d}_A\,(=D_A)$, respectively, and introduce the unit vectors $_\ell M_A$ in the direction of the reference lattice director. Then,

$$\left.\begin{aligned}
&D_A = {}_\ell M_A D_A, \quad d_A^2 = d_A\cdot d_A = D_A\cdot({}_\ell C[D_A]) \quad (\text{no sum on } A),\\
&_\ell\lambda_A^2 = d_A^2/D_A^2 = {}_\ell M_A\cdot({}_\ell C[{}_\ell M_A]) \quad (\text{no sum on } A).
\end{aligned}\right\} \tag{3.30}$$

From (3.29), we have

$$\lambda_A = \frac{ds_A}{dS_A} = \frac{ds_A}{d\bar{s}_A}\frac{d\bar{s}_A}{dS_A} = \bar{\lambda}_A\,\lambda_A^p, \tag{3.31}$$
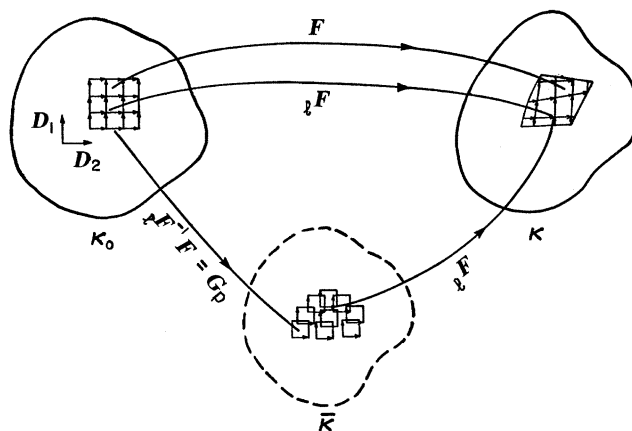
Figure 1. An exaggerated schematic diagram representing (on the macroscopic scale) the elastic–plastic deformation of a single crystal, from a reference configuration κ_0 to the current configuration κ. The deformation gradient F takes a material line element in κ_0 to a corresponding line element in κ (see $(3.4)_1$), while the lattice deformation tensor $_\ell F$ takes the lattice vectors in κ_0 to those in κ (see $(3.7)_1$). Also shown is the intermediate configuration $\bar\kappa$ depicting the tangent spaces (at each material point in κ) as representing a small neighbourhood on the microscopic scale. These tangent spaces are obtained by application of G_p to the material line elements in κ_0 (see (3.11)). Ideally the configuration $\bar\kappa$ (which is drawn by dashed lines to emphasize its local nature) should be superimposed on the current configuration κ but these would conceal the nature of physical processes on the microscopic scale. The arrows represent the lattice vectors, which are identical in the configurations κ_0 and $\bar\kappa$. The material points in the intermediate configuration $\bar\kappa$ do not continuously fit together since G_p does not satisfy the compatibility conditions. Although the lattice vectors in both κ_0 and $\bar\kappa$ are shown to be orthonormal, it should be emphasized that in general they are functions of the reference position X and need not be orthogonal, although it is difficult to depict the non-orthogonality in the diagram. Furthermore, neither κ_0 nor $\bar\kappa$ need be stress-free.

which relates the stretch λ_A to the stretch in the intermediate configuration and the plastic stretch due to G_p. It should also be observed that the second-order tensor $_\ell C$ plays a dual role: By $(3.30)_3$ is a measure of the lattice stretch $_\ell \lambda_A$ with respect to the reference lattice director in κ_0 and by $(3.29)_5$ is a measure of the purely elastic stretch $\bar\lambda_A$ in the intermediate configuration $\bar\kappa$ (see figure 1).

Our discussion in this subsection so far has dealt with measure of stretch associated with $_\ell F$, G_p and F and related formulae. A corresponding analysis of the various rotation tensors in (3.23) is much more complex; and, in general, cannot be expected to yield a simple formula analogous to (3.31). Nevertheless, under a certain restrictive condition, a relation similar to (3.31) can be deduced and this will be considered in the rest of this subsection.

Thus, consider the application of $(3.22)_2$ to the lattice deformation tensor $_\ell F$ and write

$$_\ell F = {_\ell V} {_\ell R}, \quad {_\ell V} = {_\ell R} {_\ell U} R^T, \tag{3.32}$$

where $_\ell V$ in $(3.32)_2$ is obtained from (3.22) and the fact that $R^{-1} = R^T$. With the help of both $(3.23)_1$ and $(3.23)_2$, (3.8) can be used to yield an equation in the form

$$RUU_p^{-1} = {_\ell V}R^*, \quad R^* = {_\ell R}R_p. \tag{3.33}$$

Next, multiplying the left-hand side of $(3.33)_1$ with $I = R^T R$, we may rewrite $(3.33)_1$ as

$$(RUU_p^{-1}R^T)R = {_\ell V}R^* = \bar Z \quad \text{(say)}. \tag{3.34}$$

Now with the assumption that both U and U_p have the same eigenvectors, the truth of the following results can be easily demonstrated (detailed proofs are omitted here): By writing U and U_p^{-1} in their canonical form, UU_p^{-1} is symmetric positive definite; and hence the quantity in parentheses on the left-hand side of (3.34) is also symmetric positive definite. This conclusion, in turn, implies that the second-order tensor $\bar{Z}$ in (3.34) has two left polar decompositions which is impossible by the uniqueness property of the polar decomposition theorem. It then follows from (3.34) that we must have $R^* = R$, where R^* is defined by (3.33). We may summarize the conclusion just obtained by the following:

Theorem 3.2. *The local rotation tensor R admits a multiplicative decomposition into a plastic rotation R_p and a lattice rotation $_\ell R$ in the form*

$$R = {_\ell R}R_p, \tag{3.35}$$

if and only if U and U_p have the same eigenvectors.

It is desirable to include here some remarks concerning the relationship between rate of deformation tensor D and the spin tensor W arising from $\dot{F}$ and the corresponding rate quantities arising from $_\ell\dot{F}$ and $\dot{G}_p$. Thus, analogously to the expression for the velocity gradient, $L = \dot{F}F^{-1}$ (see $(3.5)_1$), we define $_\ell L$ and L_p by

$$_\ell L = {_\ell\dot{F}}{_\ell F}^{-1}, \quad L_p = \dot{G}_p G_p^{-1}. \tag{3.36}$$

From (3.12) we may solve from $_\ell F\dot{G}_p F^{-1}$ and after observing from (3.8) that $F^{-1} = G_p^{-1}{_\ell F}^{-1}$ and also using $(3.36)_1$ and $(3.36)_2$ we obtain the formula

$$_\ell F L_p {_\ell F}^{-1} = L - {_\ell L}, \tag{3.37}$$

which relates L_p to the difference vector $(L - {_\ell L})$. The decomposition of the right-hand side of (3.37) into the symmetric and skew-symmetric parts in terms of L_p yields

$$\left.\begin{array}{l} D - {_\ell D} = \tfrac{1}{2}\{{_\ell F}L_p{_\ell F}^{-1} + {_\ell F}^{-T}L_p^T{_\ell F}\}, \\ W - {_\ell W} = \tfrac{1}{2}\{{_\ell F}L_p{_\ell F}^{-1} - {_\ell F}^{-T}L_p^T{_\ell F}\}, \end{array}\right\} \tag{3.38}$$

$_\ell D$ and $_\ell W$ represent the symmetric and skew-symmetric parts of $_\ell L$ respectively. It should be clear from $(3.38)_{1,2}$ that both $D - {_\ell D}$ and $W - {_\ell W}$ depend on L_p including its skew-symmetric part. Moreover, in view of the decompositions (3.23) and the definitions E and $_\ell E$ given by (3.26), we can readily calculate the expression for $\dot{E}$ and $_\ell\dot{E}$, namely

$$\dot{E} = FDF^T, \quad {_\ell\dot{E}} = {_\ell F}{_\ell D}{_\ell F}^T. \tag{3.39}$$

(c) *The gradient of plastic deformation and the continuous distributions of defects in a crystal*

As was noted in the opening paragraph of §1, the presence of imperfections in a crystal lattice plays a significant role in the inelastic behaviour of the material. Thus, for example, in a single crystal under high magnification (say to the order of $10^3 \times$ to $10^5 \times$) a large number of imperfections in a crystal lattice, called 'dislocations', can be seen in the form of criss-crossing lines. The motion of these dislocations gives rise to plastic (or permanent) deformation of the crystal. Moreover, the presence of arrays of dislocations have been used by Taylor (1934) to explain the hardening characteristics of a single crystal subjected to plastic deformation. In view of this vital role played by dislocations as a consequence of permanent deformation in a crystal, we need to continue our discussion of the kinematics of the lattice structure with reference to these dislocations.

Thus we begin by assuming that a single crystal possesses an ideal (or perfect) undistorted reference configuration, i.e. a reference configuration in which no lattice imperfection is present. (A configuration of this kind is referred to as a 'perfect reference lattice' by Bilby (1960, p. 337) and 'comparison crystal' by Eshelby (1956, p. 137).) It should be noted that the ideal reference configuration is not necessarily the same as the initial configuration since most crystals in their natural state possess some dislocations. In such a reference state, the lattice directors D_A coincide with the basis vectors E_A in the reference configuration. Further, since the lattice in its reference state is perfect and undistorted, there is no spatial gradient of the lattice directors with respect to X_B so that $D_{A,B} = 0$.

With the above choice of the reference configuration, we are now in a position to introduce a measure of *dislocation density*, i.e. the number of dislocation lines crossing a given area element in the current configuration of a deformed crystal. Following the procedure adopted by Bilby (1960), we define a Burgers circuit as a closed sequence of lattice steps (or segments) in a deformed crystal lattice (see the quotation (c) from Bilby 1960 in Appendix A). The corresponding steps (or segments) in the reference lattice, called the *associated* path, can be easily realized with the help of $(3.7)_2$ relating the triad of lattice directors of the reference lattice to that of the current lattice. In general, such a path is not closed, but begins at a lattice starting point S and ends at a lattice final point F (see, for example, Hirth & Lothe 1982, figs 1.20 and 1.21, pp. 22–23; Guinier 1984, fig. 5.8). We define the positive normal to the area enclosed by the Burgers circuit by the right-hand screw convention. In this way, the vector $\overrightarrow{FS}$ in the reference lattice is called the Burgers vector and is a measure of the number of dislocation lines treading the circuit.

The description in the above two paragraphs has its roots in regarding a single crystal as a discrete set of lattice points and a finite number of discrete dislocation lines. We now proceed to define the Burgers circuit and its associated path for the continuous lattice structure. For this purpose, consider a simple closed curve $\mathscr{C}$, referred to as a circuit and parametrized by $\lambda \in [0, 1]$, in the current configuration $\boldsymbol{\kappa}$ at some time t_0. The position vector of any material point on $\mathscr{C}$ is then specified by $x = \hat{x}(\lambda)$, and $\hat{x}(0)$ can be taken as the material point corresponding to the starting point S (referred to in the preceding paragraph). Further, let the closed curve $\mathscr{C}_0$ be the inverse image of $\mathscr{C}$ in the reference configuration $\boldsymbol{\kappa}_0$ such that

$$X = \hat{X}(\lambda) = \boldsymbol{\chi}^{-1}(\hat{x}(\lambda), t_0). \tag{3.40}$$

By virtue of the invertibility of $(3.1)_1$, $X = \boldsymbol{\chi}^{-1}(x, t)$ and any entity defined as a function of X can be expressed as a different function of (x, t). Applying this to the reference director triad D_A in $\boldsymbol{\kappa}_0$ and to $d_A = \mathscr{D}_A(X, t)$ in $\boldsymbol{\kappa}$, we have

$$\left. \begin{aligned} D_A &= D_A(X) = D_A[\boldsymbol{\chi}^{-1}(x, t)] = \tilde{D}_A(x, t), \\ d_A &= \mathscr{D}_A(X, t) = \mathscr{D}_A[\boldsymbol{\chi}^{-1}(x, t), t] = \tilde{d}_A(x, t). \end{aligned} \right\} \tag{3.41}$$

The right-hand sides of $(3.41)_{1,2}$ are the spatial (eulerian) representation of D_A and d_A, respectively. When a crystal is undergoing a process, the current lattice directors d_A change with time, but the material derivative of $\tilde{D}_A$ is zero.

We may associate with $\mathscr{C}$ a different curve $\mathscr{C}'$, also parametrized by λ, in the current configuration $\boldsymbol{\kappa}$ such that material points $\bar{x}(\lambda, t_0)$ on $\mathscr{C}'$ have the following properties:

$$\mathrm{d}\bar{x}(\lambda, t_0)/\mathrm{d}\lambda = {}_{\ell}\tilde{F}^{-1}(x, t_0)\,\mathrm{d}\hat{x}(\lambda, t_0)/\mathrm{d}\lambda, \quad \bar{x}(0, t_0) = \hat{x}(0), \tag{3.42}$$

where $_\ell\tilde{\boldsymbol{F}}^{-1}$ is the spatial form of $_\ell\boldsymbol{F}^{-1}(\boldsymbol{X}, t)$ given by $(3.6)_2$. The ordinary differential equation $(3.42)_1$, along with the condition $(3.42)_2$ may be viewed as an initial-value problem for which a unique solution always exists, provided that $_\ell\tilde{\boldsymbol{F}}^{-1}$ and the tangent vector $\mathrm{d}\hat{\boldsymbol{x}}/\mathrm{d}\lambda$ are sufficiently smooth (see, for example, Cartan 1983, p. 108). Several properties of $\mathscr{C}'$ must be noted: (i) The curve $\mathscr{C}'$ passes through different material points in $\boldsymbol{\kappa}$ than does $\mathscr{C}$; (ii) in general, $\mathscr{C}'$ is not closed, i.e. $\bar{\boldsymbol{x}}(0) \neq \bar{\boldsymbol{x}}(1)$; and (iii) since $\mathscr{C}'$ depends on the choice of the starting point $\hat{\boldsymbol{x}}(0)$, it is unique only up to a translation. It then follows that the difference vector $\bar{\boldsymbol{x}}(0) - \bar{\boldsymbol{x}}(1)$ is unique, depends only on $\mathscr{C}$ by $(3.42)_1$, and is independent of the choice of the starting point. We refer to the curve $\mathscr{C}'$ as the *associated path* to the circuit $\mathscr{C}$.

Preliminary to the identification of the Burgers circuit, we need to obtain an explicit analytical relationship between the paths $\mathscr{C}$ and $\mathscr{C}'$. To this end, we first observe that in the context of the continuous lattice structure, the contravariant components $\mathrm{d}\hat{x}^A$ of the increment $\mathrm{d}\hat{\boldsymbol{x}}$ referred to the lattice directors $\boldsymbol{d}_A$ are:

$$\mathrm{d}\hat{x}^A(\lambda, t_0) = \mathrm{d}\hat{\boldsymbol{x}}(\lambda, t_0) \cdot \boldsymbol{d}^A(\boldsymbol{x}(\lambda, t_0), t_0). \tag{3.43}$$

The components $\mathrm{d}\hat{x}^A$ represent the incremental distance travelled along each of the lattice vectors and hence they are the infinitesimal 'lattice step' corresponding to the 'lattice steps' in the discrete description of the lattice. Similarly, the components of $\mathrm{d}\bar{x}^A$ of the increment $\mathrm{d}\bar{\boldsymbol{x}}$ along the lattice directors $\tilde{\boldsymbol{D}}_A$ on the curve $\mathscr{C}$ are

$$\mathrm{d}\bar{x}^A(\lambda, t_0) = \mathrm{d}\bar{\boldsymbol{x}}(\lambda, t_0) \cdot \tilde{\boldsymbol{D}}^A(\hat{\boldsymbol{x}}(\lambda)) \quad (A = 1, 2, 3). \tag{3.44}$$

The components $\mathrm{d}\bar{x}^A$ are the incremental lattice steps performed in the reference lattice. In writing (3.41)–(3.44), for clarity's sake we have exhibited the dependence of $\bar{\boldsymbol{x}}$, $\hat{\boldsymbol{x}}$ (and their components) on their arguments to emphasize the curve on which these functions are evaluated. In the rest of this subsection, however, we suppress the arguments of these functions and their derivatives without ambiguity. From the relation (3.42) and $(3.7)_1$, we have

$$\mathrm{d}\bar{x}^A = {}_\ell\tilde{\boldsymbol{F}}^{-1}\,\mathrm{d}\hat{\boldsymbol{x}} \cdot \tilde{\boldsymbol{D}}^A = \mathrm{d}\hat{\boldsymbol{x}} \cdot ({}_\ell\boldsymbol{F}^{-1})^{\mathrm{T}}\,\tilde{\boldsymbol{D}}^A = \mathrm{d}\hat{\boldsymbol{x}} \cdot \tilde{\boldsymbol{d}}^A$$

and after recalling (3.43) we deduce the important result that

$$\mathrm{d}\bar{x}^A = \mathrm{d}\hat{x}^A, \tag{3.45}$$

i.e. the same number of lattice steps are performed along the curve $\mathscr{C}$ and $\mathscr{C}'$ in $\boldsymbol{\kappa}$. In view of (3.45) and recalling the definition of the Burgers vector, we may identify the difference vector $\bar{\boldsymbol{x}}(0) - \bar{\boldsymbol{x}}(1)$ as the Burgers vector and denote it by $\boldsymbol{B}$.

To relate the Burgers vector defined above to the plastic deformation we proceed with the following calculations:

$$\boldsymbol{B}(\mathscr{C}, t_0) = \bar{\boldsymbol{x}}(0, t_0) - \bar{\boldsymbol{x}}(1, t_0)$$

$$= -\int_0^1 \frac{\mathrm{d}\bar{\boldsymbol{x}}}{\mathrm{d}\lambda}\,\mathrm{d}\lambda$$

$$= -\int_0^1 {}_\ell\tilde{\boldsymbol{F}}^{-1}(\boldsymbol{x}) \frac{\mathrm{d}\hat{\boldsymbol{x}}(\lambda)}{\mathrm{d}\lambda}\,\mathrm{d}\lambda$$

$$= -\oint_{\mathscr{C}} {}_\ell\tilde{\boldsymbol{F}}^{-1}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}, \tag{3.46}$$

where in writing $(3.46)_2$ use has been made of $(3.42)_1$. The last integral in (3.46) can

be transformed into a line integral over $\mathscr{C}_0$ in $\boldsymbol{\kappa}_0$, with the help of (3.4); and, after recalling the definition of plastic strain in (3.8), yields

$$\boldsymbol{B} = -\oint_{\mathscr{C}_0} \boldsymbol{G}_{\mathrm{p}} \, \mathrm{d}\boldsymbol{X}. \tag{3.47}$$

Applying Stokes's theorem to the line integral in (3.47) we obtain

$$B(\mathscr{C}) = \int_{\mathscr{A}} \boldsymbol{\alpha}[\boldsymbol{N}] \, \mathrm{d}A, \tag{3.48}$$

where we have set

$$\boldsymbol{\alpha} = -(\operatorname{curl} \boldsymbol{G}_{\mathrm{p}})^{\mathrm{T}}. \tag{3.49}$$

In (3.48)–(3.49), $\mathrm{d}A$ is an area element, $\mathscr{A}$ is any surface area bounded by $\mathscr{C}_0$ and $\boldsymbol{N}$ is the positive normal to $\mathscr{A}$ determined by a right-hand screw rule. Also, 'curl' stands for the curl operator defined by

$$\operatorname{curl} \boldsymbol{G}_{\mathrm{p}}[\boldsymbol{a}] = \operatorname{curl}[\boldsymbol{G}_{\mathrm{p}}^{\mathrm{T}} \boldsymbol{a}] = \nabla \times (\boldsymbol{G}_{\mathrm{p}}^{\mathrm{T}} \boldsymbol{a}) \tag{3.50}$$

for any arbitrary vector $\boldsymbol{a}$, where $\nabla \equiv \partial/\partial\boldsymbol{X}$ and operates on the vector $(\boldsymbol{G}_{\mathrm{p}}^{\mathrm{T}} \boldsymbol{a})$. Then, with $\boldsymbol{a}$ set equal to $\boldsymbol{E}_A$ the components of the second-order tensor $\boldsymbol{\alpha}$ referred to the appropriate orthonormal basis reads as

$$\alpha_{AB} = \epsilon_{KBM} G^{\mathrm{p}}_{AK,M}, \quad \boldsymbol{\alpha} = \alpha_{AB} \boldsymbol{E}_A \otimes \boldsymbol{E}_B,$$

where G^{p}_{AK} denotes the components of $\boldsymbol{G}_{\mathrm{p}}$ and ϵ_{KBM} are the components of the permutation symbol.

The variable $\boldsymbol{\alpha}$ defined by (3.49) will be called the relative *dislocation density tensor*, while the vector $\boldsymbol{\alpha}[\boldsymbol{N}]$ (which occurs in the integrand of (3.48)) represents Burgers vector per unit area of the dislocations crossing a surface in $\boldsymbol{\kappa}_0$ with positive normal $\boldsymbol{N}$. Other authors, notably Eshelby (1956) and Bilby (1960), have applied Stokes's theorem to an expression analogous to (3.46) and obtained a measure of the dislocation density per unit area in the current configuration $\boldsymbol{\kappa}$ in terms of the gradient of $_{l}\boldsymbol{F}^{-1}$ with respect to the current position $\boldsymbol{x}$. It should be emphasized that our definition of the dislocation density (which differs from that in the existing literature, e.g. Eshelby 1956 and Bilby 1960) has the following features: (i) it is directly related to the gradient of plastic deformation $\boldsymbol{G}_{\mathrm{p}}$; (ii) it is measured per unit area in the reference configuration $\boldsymbol{\kappa}_0$, and relative to the reference lattice structure (here the director triad $\boldsymbol{D}_A$); and (iii) it permits the possibility that $\boldsymbol{\kappa}_0$ itself may possess dislocations, as encountered with 'as grown' crystals.

Before closing this subsection, it is desirable to comment on the relationship between our kinematical results and that usually discussed in the context of non-riemannian geometry. Several authors, beginning with Bilby *et al.* (1955) have developed a purely geometrical description of dislocations by using the methods of differential geometry of non-riemannian manifolds. In particular, they have shown that the torsion tensor of the manifold may be identified with the dislocation density per unit area in the current configuration $\boldsymbol{\kappa}$. Moreover, Bilby *et al.* (1957) have considered the closely related concept of rate of change (or 'increment') of dislocation density during deformation, while several authors (Kondo 1964; DeWit 1981; Kröner 1958, 1981) have attempted to develop a purely geometrical theory of imperfections in a crystal lattice.

All of the foregoing efforts have concentrated on using the gradient of $_{l}\boldsymbol{F}$ as the 'connection coefficient' of a non-riemannian manifold (Bilby 1960) and relating the

torsion and curvature tensors to the defectiveness of the crystals. In this regard, mention may be made of a recent paper by Davini & Parry (1991) who have discussed certain kinematical aspects of defects in a crystal and, under the restriction of defect-preserving transformation (corresponding to only elastic processes using the terminology of the present paper), have provided a list of invariants for defective crystals.

Geometrical interpretations and results of the kind mentioned in the preceding paragraph are clearly useful since the presence of defects such as impurities, which alter the structure of the lattice, may block the passage of dislocations and hence contribute to the work-hardening effects (see in this connection, Hirth & Lothe (1982, pp. 639–697) for a discussion of the interactions between dislocations and impurity atoms and Van Bueren (1961, pp. 182–219) for a description of hardening as a result of such interactions). With this background and in view of the results obtained in this subsection, Grad G_{p} may be used as a measure of the defectiveness in a crystal. Moreover, in line with remarks made in the last two paragraphs, Grad G_{p} may be used to define the 'connection coefficients' of a non-riemannian manifold, but an explicit introduction of the non-riemannian manifold is not necessary for the purposes of the present paper.

(d) *Invariance of plastic deformation tensor and dislocation density*

We recall that as a consequence of the motion specified by the vector function $\boldsymbol{\chi}$, the material point $\boldsymbol{X}$ in $\mathscr{B}$ occupies the place $\boldsymbol{x}$ in the configuration $\boldsymbol{\kappa}$. Under another motion, which differs from the given motion only by a superposed rigid body motion (henceforth referred to as SRBM), the material point X moves to $\boldsymbol{x}^+$ while the directors $\boldsymbol{d}_A$ move to $\boldsymbol{d}_A^+$ in the configuration $\boldsymbol{\kappa}^+$ at time $t^+ = t + a$, with a being a constant. It is well known that under such motions, $\boldsymbol{x}^+$, $\boldsymbol{d}_A^+$ and $\boldsymbol{F}^+$ transform as

$$\boldsymbol{x}^+ = \boldsymbol{a} + \boldsymbol{Q}\boldsymbol{x}, \quad \boldsymbol{d}_A^+ = \boldsymbol{Q}\boldsymbol{d}_A, \quad \boldsymbol{F}^+ = \boldsymbol{Q}\boldsymbol{F}, \tag{3.51}$$

where $\boldsymbol{a}$ is a vector function of time and $\boldsymbol{Q}$ is a proper orthogonal tensor function of time and hence satisfies the conditions:

$$\boldsymbol{Q}\boldsymbol{Q}^{\mathrm{T}} = \boldsymbol{Q}^{\mathrm{T}}\boldsymbol{Q} = \boldsymbol{I}, \quad \det[\boldsymbol{Q}] = 1. \tag{3.52}$$

It follows from $(3.51)_2$ that under SRBM the lattice deformation tensor $_\ell\boldsymbol{F}$ defined by (3.6) transforms as

$$_\ell\boldsymbol{F}^+ = \boldsymbol{Q}\,_\ell\boldsymbol{F}, \tag{3.53}$$

so that the right-hand side of (3.8) is

$$(_\ell\boldsymbol{F}^{-1}\boldsymbol{F})^+ = (\boldsymbol{Q}\,_\ell\boldsymbol{F})^{-1}(\boldsymbol{Q}\boldsymbol{F}) = \,_\ell\boldsymbol{F}^{-1}\boldsymbol{Q}^{-1}\boldsymbol{Q}\boldsymbol{F} = \,_\ell\boldsymbol{F}^{-1}\boldsymbol{F}.$$

Hence, under SRBM, the plastic deformation G_{p} and the relative dislocation density tensor transform as

$$G_{\mathrm{p}}^+ = G_{\mathrm{p}}, \quad \boldsymbol{\alpha}^+ = \boldsymbol{\alpha}. \tag{3.54}$$

4. The basic balance laws of the dynamical theory and related results

It is convenient at this point in our development to define certain additional quantities which occur in the balance laws to be introduced presently. The mass density $\rho_0 = \rho_0(\boldsymbol{X})$ and $\rho = \rho(\boldsymbol{X}, t)$ of $\mathscr{B}$ in the configurations $\boldsymbol{\kappa}_0$ and $\boldsymbol{\kappa}$ respectively; the stress vector $_{\mathrm{R}}\boldsymbol{t} = \,_{\mathrm{R}}\boldsymbol{t}(\boldsymbol{X}, t; \boldsymbol{N})$ and the director stress vectors $_{\mathrm{R}}\boldsymbol{m}^A$ each measured per unit area with an outward unit normal $\boldsymbol{N}$ in the reference configuration; the

external body force $\boldsymbol{b} = \boldsymbol{b}(\boldsymbol{X}, t)$ and the director body forces $\boldsymbol{\ell}^A = \boldsymbol{\ell}^A(\boldsymbol{X}, t)$ each per unit mass in the reference configuration; and the intrinsic director forces $_{\mathrm{R}}\boldsymbol{k}^A = {}_{\mathrm{R}}\boldsymbol{k}^A(\boldsymbol{X}, t)$ per unit volume in the reference configuration. We also assume that the quantities $_{\mathrm{R}}\boldsymbol{m}^A$, $\boldsymbol{\ell}^A$ and $_{\mathrm{R}}\boldsymbol{k}^A$ make no contributions to the moment of momentum. For convenience, we also define here the following set of second-order tensors, namely

$$\mathscr{L} = \boldsymbol{\ell}^A \otimes \boldsymbol{D}_A, \quad {}_{\mathrm{R}}\boldsymbol{K} = {}_{\mathrm{R}}\boldsymbol{k}^A \otimes \boldsymbol{D}_A, \quad {}_{\mathrm{R}}\boldsymbol{M} = {}_{\mathrm{R}}\boldsymbol{m}^A \otimes \boldsymbol{D}_A, \tag{4.1}$$

which will be utilized later in this section instead of $\boldsymbol{\ell}^A$, $_{\mathrm{R}}\boldsymbol{k}^A$, $_{\mathrm{R}}\boldsymbol{m}^A$.

Motivated by considerations at the microscopic level regarding the identification of the material point $\boldsymbol{x}$ with the centre of mass of the microscopic or submicroscopic region (see §2) and recalling from §3 that at a given material point the velocity of the lattice vector at time t in excess of that of the material line element which instantaneously coincides with it is given by the expressions (3.21), we assume that the kinetic energy per unit mass associated with the particle X has the form

$$\kappa = \tfrac{1}{2}\{\boldsymbol{v} \cdot \boldsymbol{v} + Y^{AB}({}_{\ell}\boldsymbol{FL}_{\mathrm{p}}\boldsymbol{D}_A) \cdot ({}_{\ell}\boldsymbol{FL}_{\mathrm{p}}\boldsymbol{D}_B)\}, \tag{4.2}$$

where in writing the above we have also used the definition $(3.36)_2$. With the help of the properties of inner product between tensors, the above expression for the kinetic energy κ can be rewritten in a more convenient form as

$$\kappa = \tfrac{1}{2}\{\boldsymbol{v} \cdot \boldsymbol{v} + \dot{\boldsymbol{G}}_{\mathrm{p}} \cdot (\mathscr{Y}[\dot{\boldsymbol{G}}_{\mathrm{p}}])\}, \tag{4.3}$$

where the inertia tensor coefficient $\mathscr{Y}$ is defined by

$$\begin{aligned}
\mathscr{Y} &= \mathscr{Y}_{ABCD}\, \boldsymbol{E}_A \otimes \boldsymbol{E}_B \otimes \boldsymbol{E}_C \otimes \boldsymbol{E}_D, \\
\boldsymbol{Y} &= Y^{AB}\, \boldsymbol{D}_A \otimes \boldsymbol{D}_B = Y_{MN}\, \boldsymbol{E}_M \otimes \boldsymbol{E}_N,
\end{aligned} \tag{4.4}$$

and where

$$\mathscr{Y}_{ABCD} = \mathscr{Y}_{CDAB} = {}_{\ell}C_{AC}(\boldsymbol{G}_{\mathrm{p}}^{-1})_{BM}(\boldsymbol{G}_{\mathrm{p}}^{-1})_{DN}\, Y_{MN}, \quad Y_{MN} = Y_{NM}. \tag{4.5}$$

It should be noted that consistent with the identification made previously for $\boldsymbol{x}$ as the centre of a microscopic region and $\boldsymbol{d}_A$ with the lattice vectors at $\boldsymbol{x}$, no coupling term involving $\dot{\boldsymbol{G}}_{\mathrm{p}}[\boldsymbol{v}]$ is admitted in the macroscopic kinetic energy in (4.1). Support for this feature of the kinetic energy can be readily provided through a derivation from a balance of energy, together with the invariance requirements under superposed rigid body motions, which demonstrates that this form of the kinetic energy (i.e. the absence of the coupling term involving $\dot{\boldsymbol{G}}_{\mathrm{p}}[\boldsymbol{v}]$) is consistent with (3.54), the invariance conditions $(4.18)_{1,2}$ below, and the invariance property of the balance of energy under superposed rigid body motions. The same derivation also provides the fact that the consequence of the moment of momentum principle does not include any contributions from the director fields and the associated kinetical quantities $({}_{\mathrm{R}}\boldsymbol{K}, {}_{\mathrm{R}}\boldsymbol{M})$. The details of such a derivation are not included here and are similar to those given by Naghdi (1972, pp. 484–486) in the context of the three-dimensional theory of classical continuum mechanics.

In view of (4.3), we define the momentum per unit mass corresponding to the velocity $\boldsymbol{v}$ and the director momentum per unit mass associated with $\dot{\boldsymbol{G}}_{\mathrm{p}}$ by

$$\partial\kappa/\partial\boldsymbol{v} = \boldsymbol{v}, \quad \partial\kappa/\partial\dot{\boldsymbol{G}}_{\mathrm{p}} = \mathscr{Y}[\dot{\boldsymbol{G}}_{\mathrm{p}}]. \tag{4.6}$$

Consistent with the identification of $\boldsymbol{x}$ and $\boldsymbol{d}_A$ with corresponding quantities in §2, we may regard the magnitude of the ordinary inertia coefficient in $(4.6)_1$ to be simply the magnitude of the inertia coefficients which this microscopic region would have had if no permanent deformation had occurred. The magnitude of the director inertia in

$(4.6)_2$ may then be interpreted as the magnitude of the additional inertia arising from the kinetic energy of the microscopic particles surrounding the centre of mass of this region which contribute to the permanent deformation processes taking place. Clearly then, these two parts may be viewed as representing the magnitudes of the ordinary and director kinetic energy, respectively, of the macroscopic particle X. Also, the physical dimensions of ρ_0, $_\mathrm{R}t$, and b are, respectively,

$$[ML^{-3}], \quad [ML^{-1}\,T^{-2}], \quad [LT^{-2}], \tag{4.7}$$

where the symbols $[L]$, $[M]$ and $[T]$ stand for the physical dimensions of length, mass and time. The physical dimensions of the vector fields $_\mathrm{R}m^A$, ℓ^A, $_\mathrm{R}k^A$ depends on the dimensions of d_A. As seen in §2, the vectors d_A have the dimensions of length and hence $_\mathrm{R}m^A$ and ℓ^A will have the same dimensions of $_\mathrm{R}t$ and b in (4.7) while $_\mathrm{R}k^A$ have the dimension of $[ML^{-1}\,T^{-2}]$ (it should be noted that if d_A is specified to be dimensionless, then the physical dimension of $_\mathrm{R}m^A$ will be $[ML^{-2}]$ corresponding to a physical dimension of a stress couple). In view of this discussion concerning the physical dimensions of $\{\ell^A, {}_\mathrm{R}k^A, {}_\mathrm{R}m^A\}$, the physical dimensions of the corresponding tensorial variables defined by (4.1) are:

$$[L] = [L^2\,T^{-2}], \quad [_\mathrm{R}K] = [_\mathrm{R}M] = [MT^{-2}]. \tag{4.8}$$

The balance laws utilized here, aside from being in lagrangian form, consist of mass balance and the ordinary momentum balance laws of classical continuum mechanics supplemented by one other, which is associated with the kinematical variable $\dot{G}_\mathrm{p}$ and which will be discussed presently. We recall here that the basic ingredients that enter the balance law associated with $\dot{G}_\mathrm{p}$ is assumed to make no contributions to the balance of moment of momentum. Thus, we first record the local forms of the ordinary conservation laws for mass, momentum and moment of momentum which hold for every material point in the reference configuration κ_0, i.e.

$$\rho_0 = \rho J, \quad \rho_0\,\dot{v} = \rho_0\,b + \operatorname{div}\boldsymbol{P}, \quad \boldsymbol{P}\boldsymbol{F}^\mathrm{T} = \boldsymbol{F}\boldsymbol{P}^\mathrm{T}, \quad {}_\mathrm{R}t = \boldsymbol{P}\boldsymbol{N}. \tag{4.9}$$

In (4.9), $\boldsymbol{P}$ is the first (non-symmetric Piola–Kirchhoff stress tensor, the notation 'div' stands for the divergence operator with respect to $\boldsymbol{X}$, $\boldsymbol{N}$ denotes the outward unit normal to any surface in κ_0 and the remaining variables were defined earlier in this section.

The additional balance law for any part $\mathscr{S}$ of the body $\mathscr{B}$ in κ_0 may be stated in words as

$$\left\{\begin{array}{l}\text{rate of change of momentum}\\ \text{associated with the rate}\\ \text{of plastic deformation}\end{array}\right\} = \left\{\begin{array}{l}\text{all forces arising}\\ \text{from (and maintaining) the}\\ \text{effect of plastic deformation}\end{array}\right\} \tag{4.10}$$

Then, in terms of the definitions introduced in (4.1), the statement for the rate of change of momentum of plastic deformation $\dot{G}_\mathrm{p}$ embodied in (4.10) for any part of the body occupying a region $\mathscr{P}_0$ bounded by a closed surface $\partial\mathscr{P}_0$ in κ_0, as a tensor equation, is

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathscr{P}_0}\rho_0\,\mathscr{Y}[\dot{G}_\mathrm{p}]\,\mathrm{d}V = \int_{\mathscr{P}_0}(\rho_0\,\mathscr{L} - {}_\mathrm{R}K)\,\mathrm{d}V + \int_{\partial\mathscr{P}_0}{}_\mathrm{R}M\,\mathrm{d}A, \tag{4.11}$$

where $\mathrm{d}V$ is an element of volume and $\mathrm{d}A$ an element of area in the fixed reference configuration κ_0.

By usual procedures and under suitable continuity assumptions, it follows from (4.11) that

$$\rho_0 \overline{\mathscr{Y}[\dot{\boldsymbol{G}}_{\mathrm{p}}]} = \rho_0 \bar{\boldsymbol{L}} - {}_{\mathrm{R}}\boldsymbol{K}, \tag{4.12}$$

where for later convenience we have also introduced the abbreviation $\bar{\boldsymbol{L}}$ by

$$\rho_0 \bar{\boldsymbol{L}} = \rho_0 \mathscr{L} + \operatorname{div} {}_{\mathrm{R}}\mathscr{M}, \quad {}_{\mathrm{R}}\boldsymbol{M} = {}_{\mathrm{R}}\mathscr{M}[\boldsymbol{N}]. \tag{4.13}$$

In (4.12)–(4.13), the third-order tensor ${}_{\mathrm{R}}\mathscr{M}$ is the director stress (associated with the lattice directors or equivalently plastic strain $\boldsymbol{G}_{\mathrm{p}}$) and is measured per unit area of surfaces in $\boldsymbol{\kappa}_0$. It should also be noted that the relationship $(4.13)_2$ is a consequence of a standard tetrahedron argument and that the last term in $(4.13)_1$ represents

$$\operatorname{div} {}_{\mathrm{R}}\mathscr{M} = {}_{\mathrm{R}}\mathscr{M}_{ABC,C}\, \boldsymbol{E}_A \otimes \boldsymbol{E}_B, \tag{4.14}$$

where ${}_{\mathrm{R}}\mathscr{M}_{ABC}$ are the components of ${}_{\mathrm{R}}\mathscr{M}$ referred to the basis vectors $\boldsymbol{E}_A$. It is natural to raise a question here regarding the physical interpretations that may be assigned to the various kinetical quantities that occur in the basic differential equations of motion $(4.9)_2$ and (4.12)–(4.13). In the case of the stress vector ${}_{\mathrm{R}}\boldsymbol{t}$ and consequently the stress tensor $\boldsymbol{P}$ in $(4.9)_2$ an *a priori* interpretation can be assigned which is meaningful for all media irrespective of the relevant applicability of the classical continuum mechanics. The same is not true for the other kinetical ingredient $({}_{\mathrm{R}}\boldsymbol{k}^A,\ {}_{\mathrm{R}}\boldsymbol{m}^A)$ and consequently $({}_{\mathrm{R}}\boldsymbol{K},\ {}_{\mathrm{R}}\boldsymbol{M})$ which occur in (4.12)–(4.13). The latter depend upon the physical nature of the problem and the choice of the additional kinematical variable such as $\boldsymbol{G}_{\mathrm{p}}$. Thus we defer further remarks on this point until the end of §6*a*, where the main features of the constitutive equations are discussed.

Within the framework of the macroscopic theory under discussion, the expression for the mechanical power P can be reduced to

$$P = \boldsymbol{S}\cdot\dot{\boldsymbol{E}} + {}_{\mathrm{R}}\boldsymbol{K}\cdot\dot{\boldsymbol{G}}_{\mathrm{p}} + {}_{\mathrm{R}}\mathscr{M}\cdot\operatorname{grad}\dot{\boldsymbol{G}}_{\mathrm{p}}, \tag{4.15}$$

where the notation 'grad' stands for the gradient operator with respect to $\boldsymbol{X}$ and $\boldsymbol{S}$ is the second (symmetric) Piola–Kirchhoff stress defined through

$$\boldsymbol{P} = \boldsymbol{FS}, \quad \boldsymbol{S} = \boldsymbol{S}^{\mathrm{T}}. \tag{4.16}$$

We have previously indicated that under SRBM, the place $\boldsymbol{x}$, the directors $\boldsymbol{d}_A$ and the tensor $\boldsymbol{G}_{\mathrm{p}}$ transform by $(3.51)_2$ and $(3.54)_1$. Now all the local conservation equations in (4.9) and (4.13) and the various fields occurring in these equations should be properly invariant under $(3.51)_1$: For example, as is well known, the stresses $\boldsymbol{P}$ and $\boldsymbol{S}$ transform according to the formulae

$$\boldsymbol{P}^+ = \boldsymbol{QP}, \quad \boldsymbol{S}^+ = \boldsymbol{S}. \tag{4.17}$$

Supplementary to (4.17), we stipulate the invariance properties

$${}_{\mathrm{R}}\mathscr{M}^+ = {}_{\mathrm{R}}\mathscr{M}, \quad {}_{\mathrm{R}}\boldsymbol{K}^+ = {}_{\mathrm{R}}\boldsymbol{K}. \tag{4.18}$$

This completes our discussion of the balance laws appropriate for the description of the motion of a crystal lattice. The balance laws (4.9)–(4.12) must be supplemented by constitutive equations for the functions $\boldsymbol{S}\ {}_{\mathrm{R}}\boldsymbol{K},\ {}_{\mathrm{R}}\mathscr{M}$ and the inertia coefficient $\boldsymbol{Y}$.

5. A general constrained theory for materials possessing an elastic range

Our main goal in this section is to construct a constrained theory of inelastic behaviour applicable to a wide range of materials, including single crystals. Such a constrained theory must necessarily be compatible with the balance laws in §4, which

must hold for all processes. For clarity's sake, we recall that the processes represented by the basic kinematical variables (see $(3.4)_1$ and (3.9)–(3.10)), i.e. $(\boldsymbol{F}, {}_\ell\boldsymbol{F})$ or equivalently $(\boldsymbol{F}, \boldsymbol{G}_\mathrm{p})$, have already been restricted (or 'constrained') through the notion of mechanical reversibility between the configurations $\boldsymbol{\kappa}$ and $\bar{\boldsymbol{\kappa}}$ (see figure 1) without an explicit specification of material behaviour on whose response a constraint may also be imposed.

We observe that for the inelastic behaviour of materials of interest here (e.g. 'rate-independent' elastic–plastic or 'rate-dependent' elastic–viscoplastic), there always exists an elastic range in which the plastic strain is constant or, more precisely, the rate of plastic strain vanishes. (For example, any process starting from rest is initially elastic and hence the 'boundary of the elastic range' delineates the elastic region.) In the light of these remarks, one may view the elastic behaviour as a special process of an elastic–plastic material for which

$$\dot{\boldsymbol{G}}_\mathrm{p} = \boldsymbol{0} \quad \text{during the reversible elastic process.} \tag{5.1}$$

Since elastic–plastic (or elastic–viscoplastic) materials exhibit elastic behaviour for part of their response, the condition (5.1) must necessarily be regarded as a constraint in the elastic range, the domain of which is not necessarily fixed.

(a) Development of a constrained theory

In previous developments of constrained theories within the scope of Cosserat continua or directed media (see Green *et al.* 1970, §6; Naghdi 1982, §§6 and 12), the constraints are assumed to hold for all possible motions and the material response is assumed to be capable of generating the necessary forces – called the constraint response – to maintain the constraint. These constraint forces may be arbitrarily large. In the present context, however, the constraint (5.1) is regarded to hold only during a part of the process and this requires the notion of a *constrained region*. Thus we assume that the constraint (5.1) is maintained as long as the constraint forces lie within a bounded closed region in the space of constraint forces, so that the constraint forces associated with (5.1) cannot be arbitrarily large.

In view of the definitions $(3.6)_{1,2}$ for the lattice deformation tensor and the relationship (3.8) between the plastic strain and the lattice deformation tensor (see also (3.9)), the triad of directors $\boldsymbol{d}_A$ are fully constrained during elastic deformations consistent with (5.1).

We now proceed to determine the effect of the constraint (5.1) on the kinetical quantities which enter the equations of motion $(4.9)_2$ and (4.12) and the mechanical power (4.15). Thus, we assume that each of the functions $(\boldsymbol{S}, {}_\mathrm{R}\boldsymbol{K}, {}_\mathrm{R}\mathscr{M})$ are determined to within an additive constraint response so that each response function such as $\boldsymbol{S}$ can be written as

$$(\,) = (\,)_\mathrm{ind} + (\,)_\mathrm{det}, \tag{5.2}$$

where the determinate parts $(\,)_\mathrm{det}$ are to be specified by constitutive equations and the indeterminate parts $(\,)_\mathrm{ind}$ are arbitrary functions of position and time and are workless. Recalling (4.15), the expression representing the worklessness of the indeterminate parts is given by

$$(\boldsymbol{S})_\mathrm{ind} \cdot \dot{\boldsymbol{E}} + ({}_\mathrm{R}\boldsymbol{K})_\mathrm{ind} \cdot \dot{\boldsymbol{G}}_\mathrm{p} + ({}_\mathrm{R}\mathscr{M})_\mathrm{ind} \cdot \mathrm{grad}\,\dot{\boldsymbol{G}}_\mathrm{p} = 0. \tag{5.3}$$

The indeterminate parts of the kinetical quantities are in general determined from (5.3) and the constraint equations in terms of Lagrange multipliers. (For a more

detailed account of constraints in the context of Cosserat continua, see §6 of Green *et al.* (1970).)

Since (5.3) must hold for every motion satisfying (5.1), by standard arguments we may conclude that

$$(_\mathrm{R}\boldsymbol{K})_\mathrm{ind} = \text{arbitrary finite}, \quad (\boldsymbol{S})_\mathrm{ind} = \boldsymbol{0}, \quad (_\mathrm{R}\mathcal{M})_\mathrm{ind} = \boldsymbol{0}. \tag{5.4}$$

In the present development, it is easily seen that the value of $(_\mathrm{R}\boldsymbol{K})_\mathrm{ind}$ can be obtained from (4.12), once constitutive equations for $(_\mathrm{R}\boldsymbol{K})_\mathrm{det}$ and $(_\mathrm{R}\mathcal{M})_\mathrm{det}$ are known, i.e.

$$(_\mathrm{R}\boldsymbol{K})_\mathrm{ind} = \rho_0\,\mathcal{L} + \mathrm{div}\,(_\mathrm{R}\mathcal{M})_\mathrm{det} - (_\mathrm{R}\boldsymbol{K})_\mathrm{det}. \tag{5.5}$$

It should be emphasized that the constraint responses (5.4) and (5.5), as well as (5.1), hold only during elastic processes.

(b) *Existence of a yield surface*

Preparatory to a general discussion of constitutive equations in §6, it is desirable to discuss the nature of some of the independent variables which may be chosen for the arguments of the various response functions, including a function whose domain represents the elastic range. It is convenient at this point to specify the abbreviations $\mathcal{U}$ and $\mathcal{W}$ for the following two sets of variables:

$$\mathcal{U} = (\boldsymbol{E}, \mathcal{W}), \quad \mathcal{W} = (\boldsymbol{G}_\mathrm{p}, \mathrm{grad}\,\boldsymbol{G}_\mathrm{p}). \tag{5.6}$$

It should also be noted that the third-order tensor $\mathrm{grad}\,\boldsymbol{G}_\mathrm{p}$ can be decomposed uniquely into a symmetric part and a skew-symmetric part according to:

$$\mathrm{grad}\,\boldsymbol{G}_\mathrm{p} = G^\mathrm{p}_{AB,\,C}\,\boldsymbol{E}_A \otimes \boldsymbol{E}_B \otimes \boldsymbol{E}_C, \quad G^\mathrm{p}_{AB,\,C} = (G^\mathrm{p}_{AB,\,C})_\mathrm{sym} + (G^\mathrm{p}_{AB,\,C})_\mathrm{skew}, \tag{5.7}$$

where the notation G^p_{AB} stands for the components of $\boldsymbol{G}_\mathrm{p}$ and a comma in $(5.7)_2$ stands for partial differentiation with respect to reference position X_C. Also the symmetric and skew-symmetric parts of $G^\mathrm{p}_{AB,\,C}$ in (5.7) are defined as

$$(G^\mathrm{p}_{ABC})_\mathrm{sym} = \tfrac{1}{2}(G^\mathrm{p}_{AB,\,C} + G^\mathrm{p}_{CB,\,A}), \quad (G^\mathrm{p}_{AB,\,C})_\mathrm{skew} = \tfrac{1}{2}(G^\mathrm{p}_{AB,\,C} - G^\mathrm{p}_{CB,\,A}). \tag{5.8}$$

Associated with $(\mathrm{grad}\,\boldsymbol{G}_\mathrm{p})_\mathrm{skew}$ is a second-order 'axial tensor' defined by (3.50), which is directly related to the dislocation density $\boldsymbol{\alpha}$ defined by (3.49).

Given the foregoing background, the use of only the variables $\mathcal{U}$ defined by (5.6) will suffice for our present purpose. We observe, however, that the inclusions of additional kinematical variables (should this become desirable) at a future occasion will not alter the basic structure of the theory presented here.

We now admit the existence of a smooth scalar-valued yield (or loading) function Φ such that for fixed values of $\mathcal{U}$ the equation

$$\Phi((_\mathrm{R}\boldsymbol{K})_\mathrm{ind}, \mathcal{U}) = 0 \tag{5.9}$$

represents a closed orientable hypersurface $\partial\mathcal{K}$ of dimensions eight, enclosing an open region $\mathcal{K}$ in the nine-dimensional $_\mathrm{R}\boldsymbol{K}$-space (see figure 2). The hypersurface $\partial\mathcal{K}$ will be called the yield surface in $_\mathrm{R}\boldsymbol{K}$-space. In view of the ideas motivated at the beginning of §5*a*, we may now stipulate that the constraint (5.1) holds as long as the constraint response $(_\mathrm{R}\boldsymbol{K})_\mathrm{ind}$ lies within the region enclosed by $\partial\mathcal{K}$, so that

$$\dot{\boldsymbol{G}}_\mathrm{p} = \boldsymbol{0} \Rightarrow \Phi((_\mathrm{R}\boldsymbol{K})_\mathrm{ind}, \mathcal{U}) \leqslant 0. \tag{5.10}$$

By usual continuity arguments, it follows that the condition (5.9) must be satisfied when $(_\mathrm{R}\boldsymbol{K})_\mathrm{ind}$ reaches a critical value at impending plastic deformation.

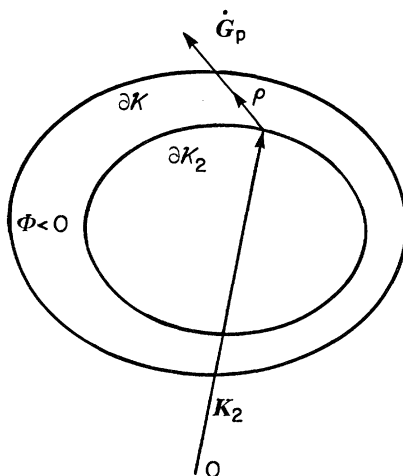Figure 2. A sketch of the yield surfaces $\partial\mathcal{K}$, $\partial\mathcal{K}_2$ and the elastic region $\Phi < 0$ in the nine-dimensional $_{\mathrm{R}}K$-space. Also shown is the unit tensor $\boldsymbol{\rho}$ representing the direction of the rate $\dot{\boldsymbol{G}}_{\mathrm{p}}$ of plastic deformation corresponding to specified value of the response function $\hat{\boldsymbol{K}}_2$; the tensor $\hat{\boldsymbol{K}}_2$ remains on the surface $\partial\mathcal{K}_2$ during plastic deformation. In general, the two surfaces $\partial\mathcal{K}$ and $\partial\mathcal{K}_2$ do not coincide and there is a jump in the value of $_{\mathrm{R}}K$ (given by (6.30)) at the initiation of yield. The two surfaces become coincident if $_{\mathrm{R}}K$ is a continuous function of time or if the inertia term in the balance equation (4.12) vanishes.

We may now construct a yield function g in the space of our basic kinematical variables corresponding to Φ in $_{\mathrm{R}}K$-space. Thus, from the left-hand side of (5.9) and using also (5.5), an expression for g can be found through the formula

$$\Phi((_{\mathrm{R}}K)_{\mathrm{ind}}, \mathcal{U}) = \Phi(\bar{L} - {}_{\mathrm{R}}\hat{K}(\mathcal{U}), \mathcal{U}) = g(\mathcal{U}; \bar{L}), \qquad (5.11)$$

where $_{\mathrm{R}}\hat{K}$ is the constitutive response function for $_{\mathrm{R}}K$ at $\dot{\boldsymbol{G}}_{\mathrm{p}} = 0$ which depends on $\mathcal{U}$ and the abbreviation $\bar{L}$ is defined by (4.13). We assume that for fixed values of $(\mathcal{W}, \bar{L})$, the equation

$$g(\mathcal{U}; \bar{L}) = 0 \qquad (5.12)$$

represents a closed orientable five-dimensional hypersurface which encloses an open region in strain space. We refer to (5.12) as the yield surface in the six-dimensional space of strain.

6. Constitutive equations for the macroscopic theory

We are concerned here with the development of constitutive equations and their restrictions in the context of the purely mechanical constrained theory of §5 for inelastic behaviour of materials which take into account the microstructural effects, both at microscopic and submicroscopic levels. Before embarking on the main objective, it is desirable to dispose of some background information pertaining to the type of restrictions that may be imposed on the constitutive response functions. Such restrictions in a purely mechanical theory can be effected in the context of more general thermomechanical results after specialization to the isothermal case. With this in mind, we appeal to the thermomechanical formulation of Green & Naghdi (1977), who postulated an entropy balance law as part of their procedure. (We may recall here that the entropy balance was originally postulated with only a limited motivation (based on the form of the energy equation for an inviscid fluid); however,

in a recent paper (Green & Naghdi 1991), it is shown that a general balance of entropy is consistent with, and can be derived from, a general balance of energy.) In the procedure of Green & Naghdi, the equation for balance of energy after combination with the balance of entropy and elimination of external heat supply and body force terms takes a reduced form which is then regarded as an identity for all processes. The lagrangian form of this reduced energy equation for the special case of isothermal deformation (temperature $\theta = $ const.) of interest here assumes the form

$$P = \rho_0 \dot{\psi} + \rho_0 \xi - \tfrac{1}{2}(\dot{\mathscr{Y}}[\dot{G}_{\mathrm{p}}]) \cdot \dot{G}_{\mathrm{p}}, \tag{6.1}$$

where the mechanical power P is defined by (4.15), ψ is specific Helmholtz free energy and ξ is a measure of energy dissipation arising from an internal generation of entropy. (The notation ξ here corresponds to $\theta\xi$ of Green & Naghdi (1977, 1991).)

(a) Constitutive equations for the constrained theory

We begin the developments of the constitutive response functions within the framework of the constrained theory discussed in §5 by introducing a scalar γ and a unit tensor ρ which designate, respectively, the magnitude and direction of the plastic strain rate $\dot{G}_{\mathrm{p}}$ defined by

$$\gamma = \|\dot{G}_{\mathrm{p}}\|, \quad \rho = \dot{G}_{\mathrm{p}}/\|\dot{G}_{\mathrm{p}}\|, \tag{6.2}$$

where the notation $\|\cdot\|$ stands for the norm. We note that

$$\dot{G}_{\mathrm{p}} = 0 \Leftrightarrow \gamma = 0, \tag{6.3}$$

while ρ is arbitrary.

In view of the presence of the last term on the right-hand side of the reduced energy equation (6.1), it is convenient to introduce a new tensor-valued variable K defined by

$$K = (_{\mathrm{R}}K)_{\mathrm{det}} + \tfrac{1}{2}\rho_0(\dot{\mathscr{Y}}[\dot{G}_{\mathrm{p}}]) \cdot \dot{G}_{\mathrm{p}}. \tag{6.4}$$

We also assume that

$$\{S, _{\mathrm{R}}\mathscr{M}\} \tag{6.5}$$

and the scalar ψ depend on the set of variables $\mathscr{U}$ defined by $(5.6)_1$ and stipulate that the constitutive assumption for K and ξ, in addition to the variables $(5.6)_1$, depend also on the variables (γ, ρ) defined by (6.2). For later reference, it is convenient to specifically indicate the constitutive forms of ψ, K and ξ as:

$$\psi = \hat{\psi}(\mathscr{U}) \tag{6.6}$$

and

$$K = \hat{K}(\mathscr{U}, \gamma, \rho), \quad \xi = \hat{\xi}(\mathscr{U}, \gamma, \rho). \tag{6.7}$$

We now introduce the constitutive assumptions such as (6.6)–(6.7) and those for the variables (6.5) into the reduced energy equation (6.1) and record the resulting equation in terms of various response functions in the form

$$(\hat{S} - \rho_0 \,\partial\hat{\psi}/\partial E) \cdot \dot{E} + (_{\mathrm{R}}\mathscr{M} - \rho_0 \,\partial\hat{\psi}/\partial \operatorname{grad} G_{\mathrm{p}}) \cdot \operatorname{grad} \dot{G}_{\mathrm{p}} + [\hat{K} - \rho_0 \,\partial\hat{\psi}/\partial G_{\mathrm{p}}] \cdot \dot{G}_{\mathrm{p}} - \hat{\xi} = 0. \tag{6.8}$$

The above equation, by the procedure of Green & Naghdi (1977), must be satisfied identically for all processes and will place restrictions on the functional dependence of the constitutive response functions.

Consider now the implication of (6.8) for special processes during which the condition (5.1) holds, i.e. for processes associated with the elastic range of

elastic–plastic materials. Thus, for processes in which $\dot{\boldsymbol{G}}_{\mathrm{p}} = \boldsymbol{0}$ (or equivalently $\gamma = 0$ by (6.3)), the third term in (6.8) vanishes and (6.8) reduces to

$$(\hat{S} - \rho_0 \, \partial \hat{\psi} / \partial E) \cdot \dot{E} + ({}_{\mathrm{R}}\hat{\mathscr{M}} - \rho_0 \, \partial \hat{\psi} / \partial \operatorname{grad} \boldsymbol{G}_{\mathrm{p}}) \cdot \operatorname{grad} \dot{\boldsymbol{G}}_{\mathrm{p}}$$
$$- \hat{\xi}(\mathscr{U}, 0, \boldsymbol{p}) = 0 \quad \text{when (5.1) holds,} \quad (6.9)$$

which is linear in the variables

$$(\dot{E}, \operatorname{grad} \dot{\boldsymbol{G}}_{\mathrm{p}}) \tag{6.10}$$

and with coefficient response functions $(\hat{S}, {}_{\mathrm{R}}\hat{\mathscr{M}}, \hat{\psi})$ which are independent of the rate quantities (6.10). Since (6.9) must hold for every choice of the variables (6.10), by standard arguments we conclude that

$$\hat{\xi}(\mathscr{U}, 0, \boldsymbol{p}) = 0, \quad \text{when } \gamma = 0 \text{ or when (5.1) holds} \tag{6.11}$$

and that

$$S = \rho_0 \, \partial \hat{\psi} / \partial E, \quad {}_{\mathrm{R}}\mathscr{M} = \rho_0 \, \partial \hat{\psi} / \partial \operatorname{grad} \boldsymbol{G}_{\mathrm{p}}. \tag{6.12}$$

Recalling our earlier remark (§3, following (3.8)) concerning the identification of $\boldsymbol{G}_{\mathrm{p}}$, we are now in a position to verify that for the fairly general constitutive equations discussed here the processes for which the lattice vectors behave as material line elements are indeed reversible; and hence the tensor $\boldsymbol{G}_{\mathrm{p}}$ defined by (3.8) can be identified as plastic deformation. For this purpose, we observe that the conclusion (6.11) for the vanishing of the rate of energy dissipation in the elastic range of the material behaviour is consistent with our constitutive assumptions and, of course, holds only when γ defined by $(6.2)_1$ vanishes. Remembering that the response functions for $(S, {}_{\mathrm{R}}\mathscr{M}, \psi)$ are independent of $\dot{\boldsymbol{G}}_{\mathrm{p}}$ (and hence independent of $\gamma, \boldsymbol{p}$), it follows from continuity arguments between the elastic range and the elastic–plastic range that the results $(6.12)_{1,2}$ holds for all processes, including those during which $\dot{\boldsymbol{G}}_{\mathrm{p}} \neq 0$.

Returning to (6.8) and after invoking the results $(6.12)_{1,2}$, we obtain an expression for $\hat{\xi}$ in terms of the response functions $\hat{K}$ and $\hat{\psi}$, i.e.

$$\hat{\xi} = [\hat{K} - \rho_0 \, \partial \hat{\psi} / \partial \boldsymbol{G}_{\mathrm{p}}] \cdot \dot{\boldsymbol{G}}_{\mathrm{p}}. \tag{6.13}$$

Motivated by the above expression for the rate of energy dissipation, the response function for $\hat{K}$ can be expressed in a more informative form. To this end, we define a new function $\tilde{K}$ through

$$\hat{K} - \rho_0 \, \partial \hat{\psi} / \partial \boldsymbol{G}_{\mathrm{p}} = \tilde{K}(\mathscr{U}, \gamma, \boldsymbol{p}) \tag{6.14}$$

and for ease of writing also introduce the notation

$$\rho_0 \, \partial \hat{\psi} / \partial \boldsymbol{G}_{\mathrm{p}} = \hat{K}_1(\mathscr{U}). \tag{6.15}$$

Next, we define a function $\hat{K}_2(\mathscr{U})$ by

$$\hat{K}_2(\mathscr{U}, \rho) = \tilde{K}(\mathscr{U}, 0, \boldsymbol{p}), \tag{6.16}$$

and further set

$$\hat{K}_3(\mathscr{U}, \gamma, \boldsymbol{p}) = \tilde{K}(\mathscr{U}, \gamma, \rho) - \hat{K}_2(\mathscr{U}, \rho). \tag{6.17}$$

Then, by (6.17) and (6.14)–(6.15), K in (6.7) can be expressed as

$$\hat{K}(\mathscr{U}, \gamma, \boldsymbol{p}) = \hat{K}_1(\mathscr{U}) + \hat{K}_2(\mathscr{U}, \boldsymbol{p}) + \hat{K}_3(\mathscr{U}, \gamma, \boldsymbol{p}), \tag{6.18}$$

Provided that

$$\hat{K}_3(\mathscr{U}, 0, \boldsymbol{p}) = 0. \tag{6.19}$$

The truth of the condition (6.19) can be easily verified from (6.18) and (6.16) when these are evaluated at zero value of γ. With (6.18) and (6.15), the rate of energy dissipation (6.13) can be rewritten as

$$\xi = (\hat{K}_2 + \hat{K}_3) \cdot \dot{\boldsymbol{G}}_{\mathrm{p}}. \tag{6.20}$$

The value of $K_2 = \hat{K}_2(\mathscr{U}, \boldsymbol{\rho})$ is undefined at $\dot{G}_p = 0$. However, since $\dot{G}_p = 0$ represents the constraint (5.1) with the constraint response (5.5), for definiteness (and without loss in generality), wet set

$$\hat{K}_2 = 0 \quad \text{whenever} \quad \dot{G}_p = 0. \tag{6.21}$$

The derived representation (6.18) for the second-order tensor K due to the intrinsic force per unit volume $_R k^A$ maintaining the movement of dislocations consists of the sum of three parts. The first of these, namely $\hat{K}_1$, represents the effect of the second-order tensor K in the elastic range of the material, while the second term on the right-hand side of (6.18) depends only on the direction of $\dot{G}_p$ (and not on its magnitude) and the third term depends on both the magnitude and direction of $\dot{G}_p$. Although there are no direct analogies between $\hat{K}_2$ and $\hat{K}_3$ with known constitutive results in standard formulations of plasticity and viscoplasticity of the past 50 years, some comments here regarding the nature of $\hat{K}_2$ and $\hat{K}_3$ may be useful. The function $\hat{K}_2$ when inverted yields an expression which is somewhat analogous to the constitutive equation for the plastic strain rate in the so-called 'rate-independent' theory of elastic–plastic materials (see §5 of Naghdi 1990). Moreover, the function $\hat{K}_3$, which depends explicitly on γ and which in accordance with (6.19) vanishes when γ tends to zero, may be regarded as a viscoplastic response. In the context of a general discussion of elastic–viscoplastic materials, however, all three response functions on the right-hand side of (6.18) must be present. With the effect of $\hat{K}_3$ suppressed, (6.18) corresponds to that in (the more usual) rate-independent elastic–plastic behaviour.

Before further consideration of related developments in this section, it is desirable to summarize the nature of the results in this subsection: The main constitutive results obtained are the constitutive equations for the stresses $(S, _R\mathscr{M})$ given by $(6.12)_{1,2}$, the constitutive equations for the intrinsic second-order tensor K given by (6.18) and the expression for the rate of energy dissipation (6.20). These constitutive equations now enable us to elaborate on the physical interpretations that may be associated with the variables $(\hat{K}, _R\mathscr{M})$ in (6.18) and $(6.12)_2$, where $\hat{K}$ has emerged from the original $_R K$ (and hence $_R k^4$) through (6.4) and $(4.1)_2$ while $_R\mathscr{M}$ has merged from the original $_R M$ (and hence $_R m^4$) through $(4.13)_2$ and $(4.1)_3$. In particular, $\hat{K}_1$ (which is a part of $\hat{K}$ in (6.18)) can be interpreted as the elastic force on the lattice defects by the surrounding material, whereas $\hat{K}_2 + \hat{K}_3$ in (6.18) represents the effect of dissipative resistance of the lattice vectors to plastic deformation. In view of the constitutive results $(6.12)_2$, $_R\mathscr{M}$ may be associated with the increase in the core energy of the defect (here the dislocation), i.e. the energy stored in the core of the defect at the atomic level with increasing defect density. With this interpretation, and observing that G_p is dimensionless, $_R M$ may be regarded as representing a 'stress-dipole' that permits the entry of a new defect into the crystal through its boundaries. In this connection, however, we note that the core energy associated with the defects is usually small and is frequently neglected in most calculations.

(b) *Geometrical interpretation of response function $\hat{K}_2$ in (6.18)*

In a nine-dimensional euclidean $\dot{G}_p$-space, the set of all possible values of the unit tensor $\boldsymbol{\rho}$ defined by $(6.2)_2$ may be represented by points on the surface of a hypersphere of unit radius with its centre at origin. Such a surface may be parametrized by eight parameters $\phi_{(i)}$ $(i = 1, 2, ..., 8)$, using, for example, the method of stereographic projection (see Levi-Civita 1926, pp. 240–241) and is similar to that for the parametrization of a sphere in a three-dimensional euclidean space by two
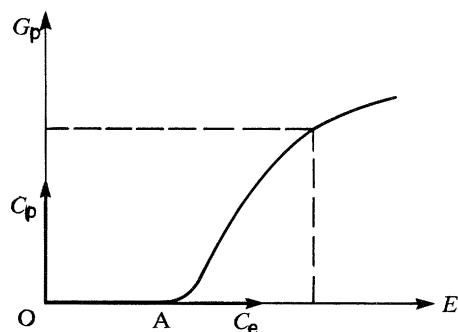
Figure 3. A schematic (two-dimensional) plot in G_p–E plane corresponding to the path of a material point in the space of the Cartesian product $E \oplus G_p$. Its projection onto the strain axis E represents a path C_e in the six-dimensional strain space, while the projection onto the plastic deformation axis G_p represents a path C_p in the nine-dimensional G_p space. The elastic range in this plot during the time interval $[t_0, t_1]$ is represented by the segment OA along the E-axis.

stereographic angles. As a result of this parametrization, any direction ρ of $\dot{G}_p$ may be specified by the values of the parameters $\phi_{(i)}$, so that $\rho = \hat{\rho}(\phi_{(i)})$. Then, the response function $\hat{K}_2$ in (6.18) may be regarded as a different function of $\mathcal{U}$ and $\phi_{(i)}$ and we may write

$$K_2 = \hat{K}_2(\mathcal{U}, \hat{\rho}(\phi_{(i)})) = \hat{K}_2(\mathcal{U}, \phi_{(i)}). \tag{6.22}$$

Since the response of K_2 for fixed values of $\mathcal{U}$ depends only on $\phi_{(i)}$, the range of $\tilde{K}_2$ in $(6.22)_2$ represents an orientable closed hypersurface of dimension eight in the nine-dimensional euclidean K_2-space. Thus, we admit the existence of a function $\Phi_2(\mathcal{U}, K_2)$ such that the equation

$$\Phi_2(\mathcal{U}, K_2) = 0 \tag{6.23}$$

for fixed values of $\mathcal{U}$ represents a hypersurface $\partial \mathcal{K}_2$ of dimension eight in the nine-dimensional euclidean K_2-space. The values of K_2 which lie on $\partial \mathcal{K}_2$ are all elements of the range of $\hat{K}_2$ (or $\tilde{K}_2$). The surface Φ_2 may be called the loading surface since the response $\hat{K}_2$ always lies on this surface during processes that give rise to plastic deformations.

A particularly simple case arises when $(6.22)_2$ involving $\tilde{K}_2$ for fixed values of the variables $\mathcal{U}$ is a one–one and differentiable function of $\phi_{(i)}$. Then, by a theorem in differential topology (Guillemin & Pollack 1974, pp. 13–18 and the theorem on p. 17), the range of $\tilde{K}_2$ is a smooth orientable compact hypersurface. (For some purposes, for example in the context of crystal plasticity, the 'one–one' or injective assumption may be too restrictive and must be relaxed but we do not discuss this issue in the present paper.)

Consider now a process at a material point X_0 in the initial configuration κ_0 of a single crystal. Let the strain trajectory (resulting from the motion χ) in strain space be denoted by C_e and designate by curve C_p the deformation of the directors at X_0 in a nine-dimensional euclidean G_p-space (see figure 3). The values of grad G_p as a function of time must also be specified for a complete description of the process, but for the time being we consider only C_e and C_p. We suppose that the deformation starting from time $t = t_0$ is initially elastic so that for $t \in [t_0, t_1]$ the plastic strain rate vanishes in accordance with (5.1). For times $t > t_1$, plastic deformation may take place, so that

$$\dot{G}_p \neq 0 \quad \text{for} \quad t > t_1. \tag{6.24}$$

By (5.1) and the discussion of the constraint in §5, it is clear that the constraint response $(_{\mathrm{R}}\boldsymbol{K})_{\mathrm{ind}}$ given by (5.5) satisfies the condition (5.9) at $t = t_1$:

$$\Phi[(_{\mathrm{R}}\boldsymbol{K}(t_1))_{\mathrm{ind}}, \mathscr{U}] = 0. \tag{6.25}$$

From (6.24) and (6.16) for $\hat{\boldsymbol{K}}_2$ follows that

$$\boldsymbol{K}_2(t > t_1) = \hat{\boldsymbol{K}}_2(\mathscr{U}(t > t_1), \boldsymbol{\rho}(t > t_1)). \tag{6.26}$$

Moreover, (6.26) satisfies

$$\Phi_2(\mathscr{U}, \boldsymbol{K}_2(t > t_1)) = 0. \tag{6.27}$$

In view of the fact that the surfaces $\partial\mathscr{K}$ and $\partial\mathscr{K}_2$ do not coincide (figure 2), there will be a jump in the value of $\ddot{\boldsymbol{G}}_{\mathrm{p}}$ at time $t = t_1$. This may be seen from the fact that as t tends to t_1 from below,

$$\lim_{t\uparrow t_1} \dot{\boldsymbol{G}}_{\mathrm{p}} = \boldsymbol{0}. \tag{6.28}$$

However, as t tends to t_1 from above, the limit of the balance law (4.12) yields

$$\ddot{\boldsymbol{G}}_{\mathrm{p}}|_{t\downarrow t_1} \boldsymbol{Y}(t_1) = -\lim_{t\downarrow t_1} \hat{\boldsymbol{K}}_2 + \rho_0 \mathscr{L}(t_1) + \mathrm{div}_{\mathrm{R}}\mathscr{M}(t_1) - \hat{\boldsymbol{K}}_1(t_1), \tag{6.29}$$

where we have assumed that $\mathscr{L}$ is continuous at $t = t_1$.

Next, after substituting for the last three terms on the right-hand side of (6.29) from (5.5) we have

$$\ddot{\boldsymbol{G}}_{\mathrm{p}}|_{t\downarrow t_1} \boldsymbol{Y}(t_1) = [_{\mathrm{R}}\boldsymbol{K}(t_1)]_{\mathrm{ind}} - \lim_{t\downarrow t_1} \hat{\boldsymbol{K}}_2(t). \tag{6.30}$$

Remembering that the coefficient $\boldsymbol{Y}$ is symmetric positive definite and hence invertible, from comparison of (6.30) and (6.28) follows the fact that $\ddot{\boldsymbol{G}}_{\mathrm{p}}$ is not continuous at $t = t_1$ unless the right-hand side of (6.30) vanishes, i.e.

$$[_{\mathrm{R}}\boldsymbol{K}(t_1)]_{\mathrm{ind}} = \lim_{t\downarrow t_1} \hat{\boldsymbol{K}}_2(t). \tag{6.31}$$

However, since $[_{\mathrm{R}}\boldsymbol{K}]_{\mathrm{ind}}$ and $\hat{\boldsymbol{K}}_2$ must respectively satisfy (6.25) and (6.27), we also have

$$\Phi[(_{\mathrm{R}}\boldsymbol{K})_{\mathrm{ind}}, \mathscr{U}] = \Phi_2[(_{\mathrm{R}}\boldsymbol{K})_{\mathrm{ind}}, \mathscr{U}]. \tag{6.32}$$

According to (6.32), the two surfaces $\partial\mathscr{K}$ and $\partial\mathscr{K}_2$ coincide and there is no distinction between the yield and loading surfaces when (6.31) holds.

(c) *A general procedure for the determination of plastic deformation and the material response*

In the development of the constitutive equations carried out in the context of the constrained theory, it was implicitly assumed that both the strain and plastic deformation trajectories C_{e} and C_{p} (see §6b) are known so that plastic deformation begins simply when $\dot{\boldsymbol{G}}_{\mathrm{p}} \neq 0$. However, in almost all cases of interest, loading history or equivalently the strain trajectory C_{e} is prescribed and part of the solution is necessarily concerned with finding the plastic deformation $\boldsymbol{G}_{\mathrm{p}}$. Here we outline a procedure by means of which the basic theory and the constitutive equations can be utilized to determine the plastic deformation trajectory C_{p} and subsequently the material response. Although not essential, for simplicity's sake, we assume that the second-order tensor $\bar{\boldsymbol{L}}$ defined by (4.13) is zero and that initially $\dot{\boldsymbol{G}}_{\mathrm{p}}$ vanishes so that initially $\Phi < 0$.

With $\bar{L} = \mathbf{0}$, the yield function g in strain space can be displayed as

$$g(\boldsymbol{E}, \mathscr{W}) = 0, \tag{6.33}$$

where the variables $\mathscr{W}$ are defined by $(5.6)_2$. In anticipation of certain results (usually referred to as loading criteria), it is convenient to introduce here a scalar $\tilde{g}$ at every point on the yield surface (6.33) defined by

$$\tilde{g} = \frac{\partial g}{\partial \boldsymbol{E}} \cdot \dot{\boldsymbol{E}} + \frac{\partial g}{\partial \operatorname{grad} \boldsymbol{G}_{\mathrm{p}}} \cdot \overline{\operatorname{grad} \boldsymbol{G}_{\mathrm{p}}}. \tag{6.34}$$

In the absence of dependence of g on $\operatorname{grad} \boldsymbol{G}_{\mathrm{p}}$, $\tilde{g}$ is identical to $\hat{g} = (\partial g/\partial \boldsymbol{E}) \cdot \dot{\boldsymbol{E}}$ which has been utilized in the strain-space formulation of plasticity for the past 15 years (see §5 of Naghdi 1990).

Now the system of governing equations consists of the mass conservation, the ordinary linear momentum and the local balance of director momenta in the form (4.12) with $\bar{L} = \mathbf{0}$, and the constitutive results for $\boldsymbol{S}$ and $\boldsymbol{K}$ given by $(6.12)_1$ and (6.18). Thus, at a given material point on a strain trajectory C_{e}, let the initial conditions at time $t = 0$ for plastic deformation $\boldsymbol{G}_{\mathrm{p}}(0)$ and $\operatorname{grad} \boldsymbol{G}_{\mathrm{p}}(0)$ be prescribed. Then, the following procedure may be used for the determination of the response of the material and the plastic deformation trajectory:

1. As the loading program is carried out, the initial response is purely elastic and no plastic deformation occurs until the yield condition (6.33) is satisfied.

2. Suppose that the condition (6.33) is first satisfied at time $t = t_1$, assume that at this instant $(t = t_1)$ plastic deformation does not set in and then examine whether or not this is compatible with the constraint condition (5.1) and the constrained theory of §5. To this end, we consider the material derivative of (6.33) evaluated at $t = t_1$ and remembering that the plastic strain does not begin at $t = t_1$, we arrive at

$$\dot{g}|_{t=t_1} = \frac{\partial g}{\partial \boldsymbol{E}} \cdot \dot{\boldsymbol{E}} + \frac{\partial g}{\partial \operatorname{grad} \boldsymbol{E}_{\mathrm{p}}} \cdot \overline{\operatorname{grad} \boldsymbol{E}_{\mathrm{p}}} = \tilde{g}, \tag{6.35}$$

where in writing the right-hand side of (6.35) we have used the notation $\tilde{g}$ defined by (6.34). We further observe that if $\tilde{g} \leqslant 0$, then in the limit as Δt tends to zero from above

$$\lim_{\Delta t \downarrow 0} \{g|_{t_1+\Delta t} = g|_{t_1} + \dot{g}|_{t=t_1} \Delta t = \tilde{g}|_{t=t_1} \Delta t\} \leqslant 0. \tag{6.36}$$

3. Given that $\tilde{g}|_{t=t_1} = 0$, then it should be clear from (6.36) that $g|_{t_1+\Delta t}$ must also be zero. This corresponds to the C_{p} trajectory moving along the hyperplane tangent to the yield surface and can be viewed as the analogue of the condition for 'neutral loading' in standard developments of plasticity for which $g = 0$, $\hat{g} = 0$.

Clearly, as long as $\tilde{g} \leqslant 0$, the assumption of absence of plastic deformation is compatible with the constraint condition (5.1), whereas $\tilde{g} > 0$ is not compatible with (5.1). Thus we may conclude that loading takes place only if

$$g = 0, \quad \tilde{g} > 0 \quad \text{for loading}. \tag{6.37}$$

4. Once plastic deformation is initiated, the various response functions may be calculated from their appropriate constitutive equations; and then the director momenta equation (4.12) with $\bar{L} = \mathbf{0}$ may be integrated to obtain the plastic deformation trajectory C_{p} as a function of time.

5. The evolution of plastic deformation continues until $\dot{\boldsymbol{G}}_p$ vanishes again. Then, the crystal will sustain additional purely elastic deformation until the loading condition (6.37) is again satisfied.

An examination of the constitutive equations for $\boldsymbol{S}$ and $\boldsymbol{K}$ reveals that when $\dot{\boldsymbol{G}}_p \neq 0$, the yield condition (6.33) does not necessarily need to be satisfied so that the so-called consistency condition in standard plasticity developments does not arise here. Further, even though in §6*b* the range of the response function $\hat{\boldsymbol{K}}_2$ was delineated by the hypersurface $\partial\mathcal{K}_2$ (or $\partial\mathcal{K}$ in view of (6.32)), the loading condition (6.37) naturally arises in the context of strain space.

Before closing this section, it may be emphasized that the general development of the material response in §6 is rate-dependent in the sense that $\boldsymbol{K}$ (but not $\boldsymbol{S}$ and $_R\mathcal{M}$) depends on the rate of $\boldsymbol{G}_p$. Further, unlike $_R\boldsymbol{K}$, the ordinary stress tensor $\boldsymbol{S}$ does not play a role in the determination of the elastic domain and hence the ideas associated with the existence of the yield function $\boldsymbol{\Phi}$. However, under special or more restrictive constitutive assumptions, the response function for $\boldsymbol{K}$ can be related to $\boldsymbol{S}$ and then the role of the latter would be similar to that of standard developments in plasticity. These topics and related ones will be discussed in Part II.

Appendix A

The purposes of this appendix is to collect a few quotations from two sources on crystal dislocations and their continuous distributions (arranged in alphabetical order by names of the authors) to provide support for the model proposed in the paper. For each listing after indicating the source, before the actual quotation, we list the page number, paragraph, and the relevant lines of quotation.

Bilby (1960)

(*a*) p. 334, para. 1, lines 9–19.

> In this process not only does the lattice undergo in general a local rotation and pure strain, but also a change in shape of the crystal, as measured by a network scribed on it, takes place. This shape deformation may, in fact, be regarded as composed of two separate changes of shape; firstly, that due to changes in the lattice (the *lattice* deformation) and secondly, that due to slip and climb processes (which do not change the *lattice*) caused by the introduction and movement of dislocations. The latter deformation we call the *dislocation* deformation. The shape, lattice and dislocation deformations may be derived and analysed for the continuously dislocated crystal, and we thus obtain a description of the plastic deformation of a continuum in terms of dislocation theory.

(*b*) p. 385, para. 1, lines 10–13

> …we have focused attention on a real solid deforming in ordinary space, that is, on the simultaneous operation of the lattice and dislocation deformations, combining to give the shape change.

(*c*) p. 335, para. 3, lines 4–7.

> A *Burgers circuit* is a closed sequence of lattice steps in the real crystal. The corresponding steps, repeated in the perfect lattice, form an *associated path* which does not, in general, close, but begins at a lattice point S and end at a lattice point F.

Nabbaro (1987)

(*a*) p. 566, para. 3, lines 1–6.

> This picture is less general than that of a Cosserat continuum, in which *two* triads of directions are associated with each point. One triad is defined, as in our present considerations, by the joins of a reference point in each cell to the corresponding reference points in neighbouring cells: the other triad is a set of vectors embedded in each cell, and transforming according to its own laws when the crystal is disturbed.

(*b*) p. 583, para. 3, lines 1–4.

> We now consider the possibility of Cosserat stresses and their possible relation to the short range stress fields of dislocations. Cosserat stresses are couples per unit area associated with the internal rotations of cells... .

(*c*) p. 505, para. 4, lines 4–11

> The general conclusion is that several of these mechanisms introduce enough resistance to ensure that the speed of a dislocation under stresses of the order usually applied in experiments is considerably less than the speed of sound. Attempts have sometimes been made to explain the contribution of dislocations to the internal friction of the material ... in terms of one particular mechanism.... It is doubtful if the theory has reached the stage at which such analyses can be relied upon.

Appendix B

We provide in this appendix the mathematical details that lead to the formula (3.13) in the main text. In part of the development in §3 (between (3.28) and (3.31)), for clarity's sake the discussion was carried out with reference to three material line elements and three directors at a given material point (compare $(3.28)_{1,2}$ with $(3.4)_1$ and $(3.11)_1$). However, for purposes of this appendix it will suffice to consider a single material line element and a single director at a given material point and then generalize the results without ambiguity to that for three directors at a given material point.

We recall that as a consequence of the motion $(3.1)_1$, a material line element $d\boldsymbol{X}$ (a tangent vector to a curve C in the reference configuration $\boldsymbol{\kappa}_0$) is transformed by the formula $(3.4)_1$ into a line element $d\boldsymbol{x}$ (a tangent vector to a curve c representing the image of C in the current configuration $\boldsymbol{\kappa}$) so that its time rate of change is given by the first of $(3.4)_2$.

Consider now some vector field $\boldsymbol{d} = \bar{\boldsymbol{d}}(\boldsymbol{x}, t)$ defined over the material points of the body $\mathscr{B}$. In view of $(3.1)_1$, $\boldsymbol{d}$ can also be expressed as a different function of the reference position $\boldsymbol{X}$ and t so that

$$\boldsymbol{d} = \hat{\boldsymbol{d}}(\boldsymbol{X}, t). \tag{B 1}$$

Focusing attention on a typical material point, $\boldsymbol{X}_0$ say, we ask what are the conditions that must be imposed on $\boldsymbol{d}_0 = \hat{\boldsymbol{d}}(\boldsymbol{X}_0, t)$ to render $\boldsymbol{d}_0$ coincident with a tangent vector to a material curve during a closed time interval $t_1 \leqslant t \leqslant t_2$. Clearly, if $\boldsymbol{d}_0$ coincides with the tangent vector to a material curve during this interval, then by the first of $(3.4)_2$ we must have

$$\dot{\boldsymbol{d}}_0 = L\boldsymbol{d}_0 \quad \text{for} \quad t_1 \leqslant t \leqslant t_2, \tag{B 2}$$

which is a necessary condition for $\boldsymbol{d}_0$ to be coincident with a tangent vector to a

material curve. We now proceed to show that (B 2) is also sufficient. To prove sufficiency, consider a vector $\boldsymbol{D}_0$ located at $\boldsymbol{X}_0$, which in terms of $\boldsymbol{d}_0$ is defined here as

$$\boldsymbol{D}_0 = \boldsymbol{F}^{-1}|_{X_0}\boldsymbol{d}_0. \tag{B 3}$$

From the material time derivative of (B 3), after using also (B 2) and $\overline{\dot{\boldsymbol{F}^{-1}}} = -\boldsymbol{F}^{-1}\boldsymbol{L}$, we have

$$\dot{\boldsymbol{D}}_0 = \overline{\dot{\boldsymbol{F}^{-1}}}\boldsymbol{d}_0 + \boldsymbol{F}^{-1}\dot{\boldsymbol{d}}_0 = -\boldsymbol{F}^{-1}\boldsymbol{L}\boldsymbol{d}_0 + \boldsymbol{F}^{-1}\boldsymbol{L}\boldsymbol{d}_0 = 0. \tag{B 4}$$

It is clear from (B 4) that $\boldsymbol{D}_0$ is independent of time during the time interval $[t_1, t_2]$ and hence must represent the dual of $\boldsymbol{d}_0$ in the reference configuration. Further, consider the image of the line $\boldsymbol{X}(\lambda) = \boldsymbol{X}_0 + \lambda\boldsymbol{D}_0$, with λ as a parameter, under the mapping $(3.1)_1$. Clearly, this image corresponds to a material curve c in the current configuration $\boldsymbol{\kappa}$ given by

$$\boldsymbol{x}(\lambda, t) = \boldsymbol{\chi}(\boldsymbol{X}_0 + \lambda\boldsymbol{D}_0, t). \tag{B 5}$$

It is easily seen that the tangent vector to c at $\lambda = 0$ is $\boldsymbol{d}_0 = \hat{\boldsymbol{d}}(\boldsymbol{X}_0, t)$ and thus c is the desired material curve. Moreover, since $\boldsymbol{D}_0$ was shown to be independent of the time interval $[t_1, t_2]$, it follows that c is material only during this interval.

It is clear from the development in the preceding paragraph that (B 2) is both necessary and sufficient for the vector $\boldsymbol{d}_0$ to be a tangent vector to a material line. Thus any vector satisfying the relation (B 2) may be referred to as a material linear element in the time interval $[t_1, t_2]$. Further, recalling the definition $(3.7)_1$ for $_\ell\boldsymbol{F}$, it follows that if all the lattice directors $\boldsymbol{d}_A$ ($A = 1, 2, 3$), at a given material point $\boldsymbol{X}_0$ become coincident with material line elements during a given time interval $[t_1, t_2]$, then each of the vectors $\boldsymbol{d}_A$ satisfy a relation of the form (B 2) and we have

$$\dot{\boldsymbol{d}}_A = {}_\ell\dot{\boldsymbol{F}}\boldsymbol{D}_A = \boldsymbol{L}\boldsymbol{d}_A = \boldsymbol{L}\,{}_\ell\boldsymbol{F}\boldsymbol{D}_A, \tag{B 6}$$

from which follows the relation $_\ell\dot{\boldsymbol{F}} = \boldsymbol{L}\,_\ell\boldsymbol{F}$ during $[t_1, t_2]$. This time interval in §3 is identified as the interval during which only reversible processes take place.

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