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K. C. Le
H. Stumpf

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KHANH CHAU LE

HELMUT STUMPF

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Abstract

The kinematics of elastoplastic bodies containing continuously distributed dislocations is developed based on the multiplicative decomposition of the total deformation and the concept of crystal reference. The problem of determining the crystal reference from the given elastic strain and dislocation density is considered. The analysis shows that the latter quantities should be referred to as the state variables, and they should be the arguments in the free energy density of the body. It is shown that the free energy density satisfies the principles of frame indifference and initial scaling indifference. Within the framework of mechanics of generalized continua, the principle of virtual work and the set of static equations are formulated for a body of this type at finite strain. The internal dynamics of dislocations is shown to be described by the model of oriented media. Governing and constitutive equations consistent with the entropy production inequality are proposed with respect to the initial and current description. A linearization procedure is carried out and a comparison with Kröner's theory is provided. Special attention is focused to the link with the macroscopic finite elastoplasticity.

Contents

Chapter 0

Introduction

It is well known that in the conventional elastoplasticity the elastic and plastic rotations are not determined uniquely. There are alternative ways to overcome this difficulty. Several authors prefer to introduce an additional constitutive equation for the so-called plastic spin (see, e.g., Mandel 1971; Dafalias 1983; Loret 1983; Onat 1984). In contrary, Stumpf & Badur (1990) and independently Nemat-Nasser (1990) proved that the plastic spin is a function depending on the plastic strain rate and, therefore, no additional constitutive equation for it can be introduced. As about an appropriate choice of a corotational rate which should enter the constitutive equations various propositions can be found in the literature (Dienes 1979; Atluri 1984; Haupt 1985; Bruhns 1991; Xia & Ellyin 1993; Schieck & Stumpf 1993,1994). An alternative way that we propose in this report is to take into account the microscopic feature of plastically deformed crystals, namely the dislocation motion, and to construct a continuum model of elastoplastic bodies at finite strain, in which the elastic and plastic rotations can be determined uniquely (see also Kondo 1952; Bilby, Bullough & Smith 1955; Bilby, Gardner & Stroh 1957; Kröner 1958,1960; Noll 1967; Wang 1967; Sedov & Berdichevsky 1967; Epstein & Maugin 1990; Le & Stumpf 1994). Two notions play a crucial role in a theory of this type: the presence of *couple stresses* due to the dislocation density and of *driving force* acting on dislocations and causing their motion.

In the theory of inelastic material behavior perhaps the most difficult and controversial concept is that of the crystal reference and the associated local relaxed intermediate configuration of an elastoplastic body (see Eckart 1948; Kondo 1952; Bilby *et al.* 1955; Bilby *et al.* 1957; Kröner 1958,1960; Noll 1967; Wang 1967; Lee 1969; Epstein & Maugin 1990; Le &

Stumpf 1993*a*). According to Kröner (1958), to unstress the body undergoing nonhomogeneous plastic flow it must be considered cut into infinitesimal elements. Intuitively, one can expect that after such a thought operation elements as crystal grains should be isomorphic to each other in some sense. Noll (1967) was the first who succeeded in translating this idea into the exact mathematical language by introducing the concept of body manifolds, local configuration, uniform reference, and material isomorphism (see also Wang 1967). Although Noll's framework is sound and rigorous, it is impossible to put the dynamic theory of continuously distributed dislocations into it because of the two following reasons. First, the uniform reference in Noll's theory is considered as a characteristics of the material, so that the internal dynamics of dislocations cannot be taken into account. Second, the presence of dislocations brings a contribution to the stored energy of the body via eigenenergy, and this leads immediately to the presence of couple stresses (Kröner 1981,1993). A possible way to overcome these difficulties is to suppose that the material to be dealt with belongs to the class of oriented media according to Toupin's definition (Toupin 1964), and consequently Noll's uniform reference defining the material isomorphism should be softened to that defining only the *crystal parallelism.*

Although physical motivations leading to the concept of crystal reference are different, one can observe the common geometric structure following from its existence. Namely, due to the crystal parallelism there exists a uniquely defined crystal connection, the torsion of which can be identified with the dislocation density (or the inhomogeneity, in Noll-Wang's terminology). Further, associated with the crystal reference there is also a Riemannian structure of the body with the induced metric and the Riemannian connection. The representation of the metric relative to the initial description can be identified with the plastic strain. The difference between the Riemannian connection and the crystal connection is defined as the contortion. Torsion and contortion determine each other.

In this report we develop a kinematical model which allows one to define appropriate strain and dislocation density measures on the body tangent bundles and on the physical translation space. Of special interest is the definition of material time derivative, and the associated relative time derivatives for spatial tensors with respect to the crystal and current references (Stumpf 1993; Le & Stumpf 1993*a*). It is interesting to note that

the time derivative relative to the current reference coincides with the Lie derivative with respect to the spatial velocity field.

From what is said above it should be clear that the problem of determining the crystal reference from the given metric and torsion is important for the finite elastoplasticity. This problem is a purely kinematical one and similar to that of determining the displacement field from the given strain field in nonlinear elasticity, with the essential difference that here the unknown is a second rank tensor field. A system of first order differential equations for the inverse elastic deformation field is derived. The integrability condition of the obtained system of equations expresses the well-known property of the crystal connection, namely, that the curvature of this connection should vanish. If this condition is fulfilled, one can integrate the system of equations along any path connecting two arbitrary points of the body which allows one to determine the inverse elastic deformation field, and then the crystal reference, provided the current reference is known. A formula is derived, which is analogous to those of Cesàro (1906) for the displacement field in linear elasticity and Pietraszkiewicz (1982) and Pietraszkiewicz & Badur (1983) in nonlinear elasticity. One may prefer to use the polar decomposition theorem to represent the elastic deformation field as the composition of rotation and stretch fields. The latter one can then be calculated from the elastic strain field with the use of linear algebra. Then the inverse elastic rotation field should satisfy a system of first order differential equations. The integrability condition of this system is examined and its solution is given in form of a tensor series. Since representations of metric and torsion relative to the initial description yield the plastic strain and the dislocation density, respectively, the problem of determining the plastic deformation and the plastic rotation from those fields is a dual one to that considered above and can be solved in a similar manner.

It is interesting to compare the linearized kinematics provided here with the well-known Kröner theory (Kröner 1958,1960). Such a linearization procedure is carried out, and the comparison shows that our linearized formulae correspond to those of Kröner.

The results obtained can be used to decide about the minimal number of state variables in finite elastoplasticity with the crystal reference subject to variation (cf. Kröner 1958,1960, Sedov & Berdichevsky 1967, Le & Stumpf

1994). In fact, since the metric and connection associated with the crystal reference are its complete characteristics, they should, therefore, play the role of the state variables and can be introduced as the arguments of the free energy density of the body. We show that the free energy density, as a function of the elastic strain and the dislocation density, satisfies the principle of frame indifference and also the principle of initial scaling indifference introduced in this report. Our development of the statics of a nonlinear body containing dislocations is based on a principle of virtual work and on this ansatz of the free energy per unit crystal volume (cf. with Sedov & Berdichevsky 1967; Kröner 1992). The classical Kröner theory (1960,1981) dealt primarily with small elastic and plastic strains. In Kröner (1992) some propositions were made concerning the dependency of the free energy density on the elastic deformation and the dislocation density, while in Kröner (1993) the balance equations of micromomentum are investigated. By using the multiplicative decomposition of the deformation gradient into elastic and plastic parts we account for all degrees of freedom of macro- and micro-motion. The material containing dislocations can be considered as the one belonging to the class of oriented continua in Toupin's sense (Toupin 1964, see also the somewhat similar continuum with internal degrees of freedom proposed by Sedov & Berdichevsky 1967). But in one aspect our theory differs essentially from that of Toupin, namely our stored energy density enjoys an additional invariance with respect to the rescaling group. This leads to the balance equations of micromomentum and moment of micromomentum. The microstresses should be balanced by the internal driving force acting on the dislocations. The latter one is shown to be the sum of Eshelby's force on dislocations due to the surrounding elastic field (Eshelby 1951, Epstein & Maugin 1990) and of an additional term characterizing the interaction between dislocations. This driving force is familiar for specialists working in phase transition theory (Truskinovsky 1987; Knowles & Abeyaratne 1990) and nonlinear fracture mechanics (Stumpf & Le 1990,1992; Le & Stumpf 1993*b*; Maugin & Trimarco 1992).

Within the framework of mechanics of generalized continua (Toupin 1964; Sedov & Berdichevsky 1967) we formulate a set of balance equations and entropy production inequality in integral form for an arbitrary volume of the initial configuration. Equivalent sets of equations relative to

the current reference for a body with continuously distributed dislocations at finite strain are obtained. The entropy production inequality formulated relative to the initial reference is used to derive new constitutive equations. Equivalent sets of constitutive equations relative to the current reference are presented. We analyze special cases and show that our theory reduces to that of Noll (1967) and Wang (1967) if the crystal reference is not subject to variation. The linearized theory is shown to coincide with that of Kröner (1958, 1960). Special attention is focused to outline the connection of our theory with engineering elastoplasticity, (see, e.g., Le & Stumpf 1993*a*). In this special case our stored energy density does not depend on the dislocation density and, therefore, the couple stresses are shown to vanish.

Chapter 1

Kinematics

1.1 Preliminaries and conventions

We shall denote the three-dimensional Euclidean space by $\mathcal{E}$. Elements $x, y, \ldots$ of $\mathcal{E}$ are called spatial points. The translation space of $\mathcal{E}$ is denoted by $\mathcal{V}$; it is a three-dimensional vector space. Elements $\mathbf{u}, \mathbf{v}, \ldots$ of $\mathcal{V}$ are called spatial vectors. The inner product of two spatial vectors $\mathbf{u}, \mathbf{v} \in \mathcal{V}$ is denoted by $\mathbf{g}(\mathbf{u}, \mathbf{v})$ (sometimes by $\mathbf{u} \cdot \mathbf{v}$). One can say that $\mathbf{g}$ is the spatial metric defined on $\mathcal{V}$. The dual space of $\mathcal{V}$ is denoted by $\mathcal{V}^*$. The metric $\mathbf{g}$ establishes an isomorphism from $\mathcal{V}$ to $\mathcal{V}^*$, but we do not use this isomorphism to identify $\mathcal{V}^*$ with $\mathcal{V}$. The vector product of two spatial vectors $\mathbf{u}, \mathbf{v}$ is denoted by $\mathbf{u} \times \mathbf{v}$.

The tensor space on $\mathcal{V}$, contravariant of rank r and covariant of rank s is denoted by $T^r_s(\mathcal{V})$; its elements are denoted by boldface letters. In particular, $T^1_1(\mathcal{V})$ is the set of linear transformations of $\mathcal{V}$ into itself. The identity transformation on $\mathcal{V}$ is denoted by $\mathbf{1}$. In some cases we represent tensors also in component form, using for simplicity rectangular Cartesian co-ordinates. Unless otherwise specified, upper, lower and Greek indices take the values 1,2,3; the Einstein summation convention over repeated indices is used.

Let $\mathcal{U}$ be some open subset of $\mathcal{E}$. A map $\mathbf{t} : \mathcal{U} \to T^r_s(\mathcal{V})$ is called a tensor field (contravariant of rank r and covariant of rank s) defined on $\mathcal{U}$. The tensor field $\mathbf{t}$ is said to be of class C^1 if there is a tensor field $d\mathbf{t} : \mathcal{U} \to T^r_{s+1}(\mathcal{V})$ such that

$$\mathbf{t}(x + \mathbf{u}) = \mathbf{t}(x) + (d\mathbf{t}(x))\mathbf{u} + \epsilon(x, \mathbf{u}), \quad x \in \mathcal{U}, \mathbf{u} \in \mathcal{V},$$

where

$$\lim_{|\mathbf{u}|\to 0} \frac{1}{|\mathbf{u}|}\boldsymbol{\epsilon}(x,\mathbf{u}) = \mathbf{0}$$

holds for all $x \in \mathcal{U}$. The tensor field $d\mathbf{t}$, if it exists, is uniquely determined by $\mathbf{t}$ and is called the derivative of $\mathbf{t}$.

We assume the reader is familiar with the tensor analysis on manifolds (standard texbooks such as Abraham, Marsden & Ratiu 1988, or Sternberg 1983 could be recommended). Let $\mathcal{M}$ be a differentiable manifold. The tangent space attached to the point $X \in \mathcal{M}$ is denoted by $T_X\mathcal{M}$ and the tangent bundle on $\mathcal{M}$ by $T\mathcal{M}$. Let $\mathcal{N}$ be another differentiable manifold, and $\phi : \mathcal{M} \to \mathcal{N}$ be a differentiable map. The tangent of the map ϕ is the linear transformation from $T\mathcal{M}$ to $T\mathcal{N}$ denoted by $T\phi : T\mathcal{M} \to T\mathcal{N}$. Let E, F be two vector spaces and $\varphi : E \to F$ a linear transformation. The transpose of φ, denoted φ^T, is the linear map between dual spaces F^*, E^*, $\varphi^T : F^* \to E^*$, defined by $< \varphi^T(\boldsymbol{\beta}), \mathbf{u} >=< \boldsymbol{\beta}, \varphi(\mathbf{u}) >$, where $\boldsymbol{\beta} \in F^*$, $\mathbf{u} \in E$, and $< .,. >$ denotes the pairing between dual tensors. Throughout this paper we shall use boldface letters for vectors and tensors defined on the space $\mathcal{V}$, gothic boldface letters for vectors and tensors defined on the body manifold, and letters like $\mathbb{K}, \mathbb{H}, \ldots$ for two-point tensors. Although it is not absolutely necessary, we shall nevertheless distinguish tensors defined on $\mathcal{E}$ by ascribing upper case letters to those defined on the initial configuration, lower case ones to those on the current configuration, and lower case letters with a superposed bar to those defined on the current relaxed intermediate configuration (see the subsequent sections). The space $\mathcal{V}^*$ will not be identified with $\mathcal{V}$, for the pull-back operation applied to covariant and contravariant spatial tensors leads to different tensors on the body manifold (see Abraham *et al.* 1983).

1.2 Bodies, motions and references

In order to model elastoplastic bodies containing dislocations we shall use the concept of manifolds. We begin by identifying a body with a differentiable manifold $\mathcal{B}$ (of dimension 3). Material points in $\mathcal{B}$ are denoted $X, Y, \ldots$ A motion of $\mathcal{B}$ is a one-parameter family of placements or maps $\phi_t : \mathcal{B} \to \mathcal{E}$ specified by

$$x = \phi(X,t), \quad X \in \mathcal{B}, x \in \mathcal{E}. \tag{2.1}$$

The map ϕ is supposed to be one-to-one and as many times continuously differentiable as required. The tangent of ϕ at X, denoted by $\mathbb{K}_X = T\phi\,|_X$ and called the distortion, is the linear transformation from $T_X\mathcal{B}$ to $\mathcal{V}$. Of central importance is Noll's concept of a local configuration at X (Noll 1967), which can be defined as an equivalence class of placements with the same distortion at X. The distortion $\mathbb{K}_X$ can be considered as a representative of this class. A function $\mathbb{K}$ on $\mathcal{B}$ whose values are local configurations is called a reference for $\mathcal{B}$. If there exists a global placement ϕ such that the reference $\mathbb{K}$ can be identified with $T\phi$, we call $\mathbb{K}$ a description for $\mathcal{B}$. In the opposite case $\mathbb{K}$ will be called an anholonomic reference.

Two important examples of descriptions are: $\mathbb{K}_t = T\phi_t$ (current or Eulerian description) and $\mathbb{K}_0 = T\phi_0$ (initial or Lagrangian description). The relation between them is

$$\mathbb{K}_t = \mathbf{F}\mathbb{K}_0, \tag{2.2}$$

where $\mathbf{F}$ is the total deformation of the body. Since ϕ is supposed to be one-to-one, the deformation $\mathbf{F}$ is invertible. Moreover, we assume that

$$J = \det \mathbf{F} > 0,$$

so that $\mathbf{F}$ is the orientation preserving deformation field.

The specific feature of an elastoplastic body is that the total deformation $\mathbf{F}$ cannot fully characterize its stress state. In fact, let us consider a body undergoing nonhomogeneous plastic deformation, and let us imagine the following thought experiment (Gedankenexperiment): cut the deformed body into infinitesimal elements and reduce the stresses to zero via elastic deformations. If the plastic deformation were absent, after such a thought experiment the elements would form an unloaded initial configuration. In this case the total deformation $\mathbf{F}$ would characterize fully the stress state of the deformed body. Due to the plastic deformation the elements would not, in general, come back to the unloaded initial state, but rather to some intermediate relaxed state. Two remarks should be said about this relaxed state. First, the relaxed state depends strongly on how the elements are plastically deformed. Second, the elements after comming to the relaxed state will no longer form any viable configuration. One can speak about incompatibility due to the inhomogenous plastic deformation.

From the microscopical point of view, the relaxed state can be realized only if atoms in the Bravais crystal are in correspondance with points

of a perfect lattice (except for small thermal vibrations of atoms about these positions). Figure 1 depicts a perfect lattice (without defects) in the two-dimensional case, where the lattice points (atoms) are related by the translation vector $m\mathbf{e}_1 + n\mathbf{e}_2$, with $m, n = 1, 2, \ldots$ One can assign the zero level of free energy to this state. Due to the defect-free arrangement of the atoms one can also translate parallelly vectors in a natural way. Therefore, one expects that equal loadings applied to the elements in the relaxed state should lead to equal deviations from it.

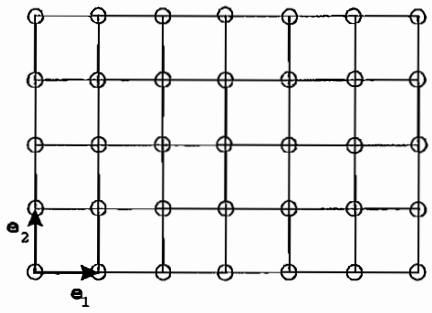

Figure 1.1: A perfect lattice

From what is said above one can see the necessity of knowing the relaxed states of the elements in order to be able to characterize fully their behaviour. This is the physical motivation for us to introduce now an (instantaneous) crystal reference $\bar{\mathbb{K}}_t$ [1], which is anholonomic and time-dependent in general, with the property that $\Phi(X, Y) = \bar{\mathbb{K}}_t^{-1}(X)\bar{\mathbb{K}}_t(Y)$ defines a *crystal parallelism* (some authors prefer the word teleparallelism) of $T_Y\mathcal{B}$ onto $T_X\mathcal{B}$ for any $X, Y \in \mathcal{B}$. Equivalently saying, $\mathbf{c} = \bar{\mathbb{K}}_t^{-1}\mathbf{c}$ is a crystallographically constant vector field for every constant vector $\mathbf{c} \in \mathcal{V}$. We assume the following relations between the references (see Fig.2)

$$\mathbb{K}_t = \mathbf{F}^e\bar{\mathbb{K}}_t, \tag{2.3}$$

$$\bar{\mathbb{K}}_t = \mathbf{F}^p\mathbb{K}_0, \tag{2.4}$$

where $\mathbf{F}^e, \mathbf{F}^p$ are the elastic and plastic deformation, respectively [2]. These tensor fields are supposed to be as many times continuously differentiable

[1] In engineering language, the local configuration $\bar{\mathbb{K}}_{tX}$ is called the local current relaxed intermediate configuration.

[2] Strictly speaking, we should have $\bar{\mathbb{K}}_t = \mathbf{F}_t^p\bar{\mathbb{K}}_0, \bar{\mathbb{K}}_0 = \mathbf{F}_0^p\mathbb{K}_0$, with $\mathbf{F}_0^p$ being the initial plastic deformation, and $\mathbf{F}^p = \mathbf{F}_t^p\mathbf{F}_0^p$. Because $\mathbf{F}_0^p$ should be given *a priori*, without loss of generality we can assume that $\mathbf{F}_0^p = \mathbf{1}$. The elastic and plastic deformations, as well as the crystal reference itself, may in general depend on the

as required. Furthermore, they should satisfy the following natural requirements

$$J^p = \det \mathbf{F}^p > 0, \quad J^e = \det \mathbf{F}^e > 0.$$

This means that $\mathbf{F}^p$ and $\mathbf{F}^e$ are orientation preserving deformation fields. Consequently, they have inverse deformation fields, denoted by $\mathbf{F}^{p-1}$ and $\mathbf{F}^{e-1}$, respectively. From (2.2)-(2.4) the multiplicative decomposition of the total deformation follows (see Figure 2)

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p. \tag{2.5}$$

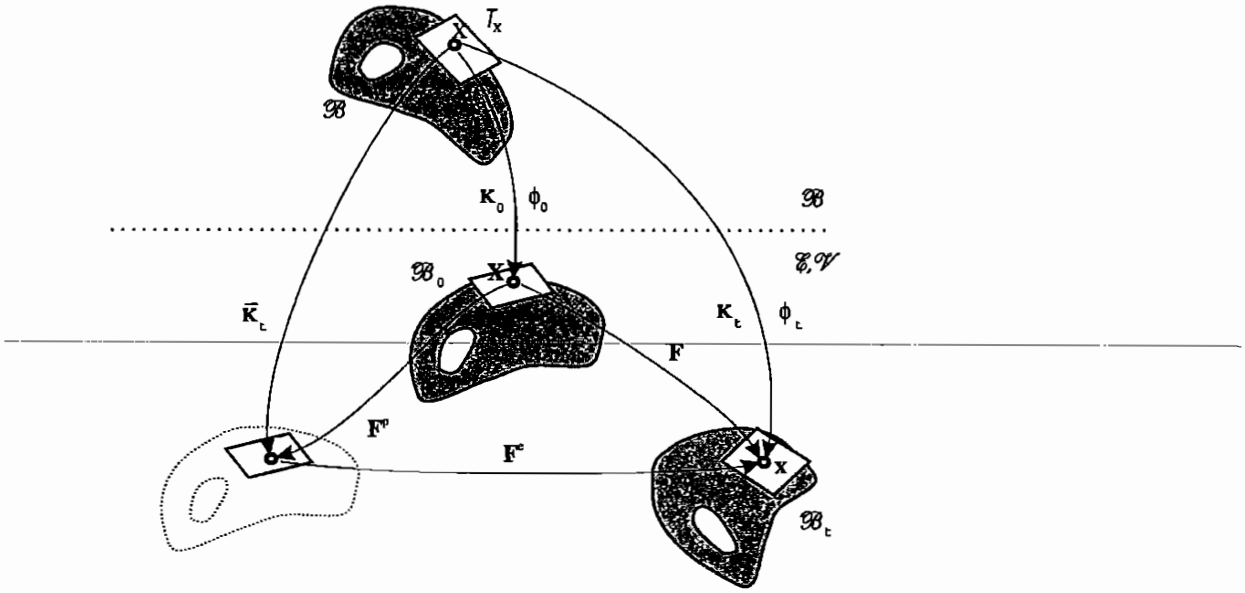

Figure 1.2: Schematic sketch of the body manifold $\mathcal{B}$, initial $\mathbb{K}_0$, crystal $\bar{\mathbb{K}}_t$, and current $\mathbb{K}_t$, references and the associated multiplicative decomposition of the total deformation.

The decomposition (2.5) was first introduced by Bilby *et al.* (1957) as a basic assumption to derive the kinematics of dislocations. In that paper (Bilby *et al.* 1957) $\mathbf{F}, \mathbf{F}^e, \mathbf{F}^p$ were called the shape deformation, the lattice deformation, and the dislocation deformation, respectively. We adopt here the terminology used by Kröner (1958,1960) and Lee (1969), who required also the independency of the free energy density from the plastic deformation in order to derive adequate constitutive equations for elastoplastic bodies at finite strain.

temperature. Since the dynamics and thermodynamics will be considered later in Chapters 4 and 5, here and in Chapters 2 and 3 we restrict ourself to isothermal processes.

1.3 Connection, torsion and curvature

Let $\mathbf{t} : \mathcal{B} \to T^r_s(\mathcal{V})$ be a mapping from $\mathcal{B}$ to the tensor space $T^r_s(\mathcal{V})$ on $\mathcal{V}$ (contravariant of rank r and covariant of rank s), and let $\mathbb{K} = d\phi$ for some ϕ. Given a description $\mathbb{K} = T\phi$ we can then introduce

$$d_{\mathbb{K}}\mathbf{t} : \mathcal{B} \to T^r_{s+1}(\mathcal{V}),$$

called the derivative of $\mathbf{t}$ relative to $\mathbb{K}$, which is defined by

$$d_{\mathbb{K}}\mathbf{t} = d(\mathbf{t} \circ \phi^{-1}) \circ \phi, \tag{3.1}$$

with d being the standard derivative for tensor fields on the vector space $\mathcal{V}$. If $\bar{\mathbb{K}}$ is anholonomic, then the derivative relative to $\bar{\mathbb{K}}$ can be defined as follows

$$d_{\bar{\mathbb{K}}}\mathbf{t} = d_{\mathbb{K}}\mathbf{t}(\mathbb{K}\bar{\mathbb{K}}^{-1}), \tag{3.2}$$

where $\mathbb{K}$ is an arbitrary description. Of course this definition is independent of the choice of $\mathbb{K}$.

In order to make the report self-contained we recall some facts from the differential geometry (see Sternberg 1983, Abraham *et al.* 1988). Let $\mathbf{w} \in T\mathcal{B}$ be a vector field and f be a function on $\mathcal{B}$. The derivative of f in the direction $\mathbf{w}$ is defined as follows

$$\mathbf{w}[f] = (d_{\mathbb{K}}f)(\mathbb{K}\mathbf{w}). \tag{3.3}$$

It is easy to prove the following properties

$$\mathbf{w}[f+g] = \mathbf{w}[f] + \mathbf{w}[g], \quad \mathbf{w}[fg] = f\mathbf{w}[g] + g\mathbf{w}[f]. \tag{3.4}$$

Actually, any vector field $\mathbf{w}$ can be identified with a mapping $f \mapsto \mathbf{w}[f]$ satisfying (3.4). Let $\mathbf{w}_1$ and $\mathbf{w}_2$ be two vector fields on $\mathcal{B}$. The Lie bracket of $\mathbf{w}_1$ and $\mathbf{w}_2$ is defined by means of the commutator:

$$[\mathbf{w}_1, \mathbf{w}_2][f] = \mathbf{w}_1[\mathbf{w}_2[f]] - \mathbf{w}_2[\mathbf{w}_1[f]]. \tag{3.5}$$

The Lie bracket of two vector fields can be identified with the vector field given by

$$[\mathbf{w}_1, \mathbf{w}_2] = \mathbb{K}^{-1}[d_{\mathbb{K}}(\mathbb{K}\mathbf{w}_2)\mathbb{K}\mathbf{w}_1 - d_{\mathbb{K}}(\mathbb{K}\mathbf{w}_1)\mathbb{K}\mathbf{w}_2],$$

where $\mathbb{K}$ is an arbitrary description. The Lie bracket satisfies the identities

$$[\mathbf{w}_1, \mathbf{w}_2] = -[\mathbf{w}_2, \mathbf{w}_1],$$

$$[\mathbf{w}_1, f\mathbf{w}_2] = f[\mathbf{w}_1, \mathbf{w}_2] + \mathbf{w}_1[f]\mathbf{w}_2,$$

$$[[\mathbf{w}_1, \mathbf{w}_2], \mathbf{w}_3] + [[\mathbf{w}_3, \mathbf{w}_1], \mathbf{w}_2] + [[\mathbf{w}_2, \mathbf{w}_3], \mathbf{w}_1] = 0 \quad \text{(Jacobi)}.$$

Let us define a connection on $\mathcal{B}$ as an operation $\nabla : T\mathcal{B} \times T\mathcal{B} \to T\mathcal{B}$ that associates to each pair of vector fields $\mathbf{w}_1, \mathbf{w}_2$ on $\mathcal{B}$ a third vector field denoted $\nabla_{\mathbf{w}_1}\mathbf{w}_2$ and called the covariant derivative of $\mathbf{w}_2$ along $\mathbf{w}_1$, such that

1. $\nabla_{\mathbf{w}_1}\mathbf{w}_2$ is linear in each of $\mathbf{w}_1$ and $\mathbf{w}_2$,
2. $\nabla_{f\mathbf{w}_1}\mathbf{w}_2 = f\nabla_{\mathbf{w}_1}\mathbf{w}_2$ for any scalar function f,
3. $\nabla_{\mathbf{w}_1}(f\mathbf{w}_2) = f\nabla_{\mathbf{w}_1}\mathbf{w}_2 + (\mathbf{w}_1[f])\mathbf{w}_2$.

Note that the third rule is analogous to the product rule for differentiation.

The Cartan torsion of a connection ∇ is a (1,2)-tensor $\mathbf{t} : T\mathcal{B} \times T\mathcal{B} \to T\mathcal{B}$ defined by

$$\mathbf{t}(\mathbf{w}_1, \mathbf{w}_2) = \nabla_{\mathbf{w}_1}\mathbf{w}_2 - \nabla_{\mathbf{w}_2}\mathbf{w}_1 - [\mathbf{w}_1, \mathbf{w}_2]. \tag{3.6}$$

From this definition it is obvious that $\mathbf{t}$ is skew-symmetric in the sense that

$$\mathbf{t}(\mathbf{w}_1, \mathbf{w}_2) = -\mathbf{t}(\mathbf{w}_2, \mathbf{w}_1).$$

We call a connection torsion-free, when its torsion tensor vanishes.

The curvature tensor of a connection ∇ is a (1,3)-tensor $\mathbf{r} : T\mathcal{B} \times T\mathcal{B} \times T\mathcal{B} \to T\mathcal{B}$, where

$$\mathbf{r}(\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3) = \nabla_{\mathbf{w}_1}\nabla_{\mathbf{w}_2}\mathbf{w}_3 - \nabla_{\mathbf{w}_2}\nabla_{\mathbf{w}_1}\mathbf{w}_3 - \nabla_{[\mathbf{w}_1,\mathbf{w}_2]}\mathbf{w}_3. \tag{3.7}$$

It is obvious that $\mathbf{r}$ is skew-symmetric as well in the sense that

$$\mathbf{r}(\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3) = -\mathbf{r}(\mathbf{w}_2, \mathbf{w}_1, \mathbf{w}_3).$$

There is an important relation between the torsion and the curvature of a connection. Namely, they satisfy Bianchi's identity

$$\sum_{cyclic} \{\nabla_{\mathbf{w}_3}(\mathbf{t}(\mathbf{w}_1, \mathbf{w}_2)) + \mathbf{t}(\mathbf{w}_2, [\mathbf{w}_3, \mathbf{w}_1]) - \mathbf{r}(\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3)\} = 0. \tag{3.8}$$

To see this, let us apply $\nabla_{\mathfrak{w}_3}$ to (3.6) which gives

$$\nabla_{\mathfrak{w}_3}(\mathfrak{t}(\mathfrak{w}_1,\mathfrak{w}_2)) - \nabla_{\mathfrak{w}_3}\nabla_{\mathfrak{w}_1}\mathfrak{w}_2 + \nabla_{\mathfrak{w}_3}\nabla_{\mathfrak{w}_2}\mathfrak{w}_1 + \nabla_{\mathfrak{w}_3}[\mathfrak{w}_1,\mathfrak{w}_2] = 0.$$

The cyclic sum of the left-hand side of this equation remains unchanged if the third term is changed by one and the fourth term by two cyclic permutations of $\mathfrak{w}_1, \mathfrak{w}_2, \mathfrak{w}_3$. Hence, we have

$$\sum_{cyclic} \{\nabla_{\mathfrak{w}_3}(\mathfrak{t}(\mathfrak{w}_1,\mathfrak{w}_2)) - \nabla_{\mathfrak{w}_3}\nabla_{\mathfrak{w}_1}\mathfrak{w}_2 + \nabla_{\mathfrak{w}_3}\nabla_{\mathfrak{w}_2}\mathfrak{w}_1 + \nabla_{\mathfrak{w}_3}[\mathfrak{w}_1,\mathfrak{w}_2]\}$$

$$= \sum_{cyclic} \{\nabla_{\mathfrak{w}_3}(\mathfrak{t}(\mathfrak{w}_1,\mathfrak{w}_2)) - [\nabla_{\mathfrak{w}_3},\nabla_{\mathfrak{w}_1}]\mathfrak{w}_2 + \nabla_{\mathfrak{w}_2}[\mathfrak{w}_3,\mathfrak{w}_1]\} = 0.$$

Using the definitions (3.6) and (3.7) we obtain

$$\sum_{cyclic} \{\nabla_{\mathfrak{w}_3}(\mathfrak{t}(\mathfrak{w}_1,\mathfrak{w}_2)) - \mathfrak{r}(\mathfrak{w}_1,\mathfrak{w}_2,\mathfrak{w}_3)$$

$$+\mathfrak{t}(\mathfrak{w}_2,[\mathfrak{w}_3,\mathfrak{w}_1]) + [\mathfrak{w}_2,[\mathfrak{w}_3,\mathfrak{w}_1]]\} = 0.$$

Due to the Jacobi identity the last term gives no contribution and (3.8) results.

Let ∇ and ∇^* be two connections on $\mathcal{B}$. From the definition of connection it is easy to see that the difference

$$\mathfrak{d} = \nabla - \nabla^*$$

can be identified with a (1,2)-tensor field on $\mathcal{B}$. We shall see later that this difference depends only on the Christoffel symbols of the connections.

1.4 Crystal connection and the dislocation density

Let us consider again the crystal reference $\bar{\mathbb{K}}_t$. We say that a vector field $\mathbf{c}$ on $\mathcal{B}$ is crystallographically constant with respect to $\bar{\mathbb{K}}_t$ if

$$\bar{\mathbb{K}}_t\mathbf{c} = \mathbf{c} = \text{const} \quad \text{with} \quad \mathbf{c} \in \mathcal{V}.$$

This vector field is the pull back of the constant spatial vector $\mathbf{c}$ by $\bar{\mathbb{K}}_t^{-1}$ at some point Y followed by the parallel translation $\bar{\mathbb{K}}_t^{-1}(X)\bar{\mathbb{K}}_t(Y)$ to all points of the body manifold (teleparallelism). We are looking now for a

connection $\bar{\nabla}$ such that $\bar{\nabla}_{\mathfrak{w}}\mathbf{c} = \mathbf{0}$ holds for an arbitrary constant vector field $\mathbf{c}$ and an arbitrary vector field $\mathfrak{w}$. Such a connection is called a crystal connection. We show that it is uniquely determined by $\bar{\mathbb{K}}_t$ according to (Noll 1967; Wang 1967)

$$\bar{\nabla}_{\mathfrak{w}_1}\mathfrak{w}_2 = \bar{\mathbb{K}}_t^{-1} d_{\bar{\mathbb{K}}_t}(\bar{\mathbb{K}}_t\mathfrak{w}_2)\bar{\mathbb{K}}_t\mathfrak{w}_1, \tag{4.1}$$

for arbitrary vector fields $\mathfrak{w}_1$ and $\mathfrak{w}_2$ on $\mathcal{B}$. First of all, we show that this definition has all the necessary properties. It is easy to see that $\bar{\nabla}_{\mathfrak{w}}\mathbf{c} = 0$ when $\mathbf{c}$ is constant, because $\mathbb{K}_t\mathbf{c} = \mathbf{c} = \text{const}$. The linearity in $\mathfrak{w}_1$ and $\mathfrak{w}_2$ is also obvious, and the product rules follow from the validity of the analogous rules for the relative derivative.

To prove the uniqueness, let us assume that ∇' is another crystal connection. Putting $\mathfrak{d}_{\mathfrak{w}} = \bar{\nabla}_{\mathfrak{w}} - \nabla'_{\mathfrak{w}}$, we then have $\mathfrak{d}_{\mathfrak{w}}\mathbf{c} = 0$ for all constant vector fields $\mathbf{c}$. We have seen at the end of the previous section that $\mathfrak{d}_{\mathfrak{w}}$ can be identified with a tensor field. Since $\mathbf{c}$ is arbitrary, we conclude that $\mathfrak{d}_{\mathfrak{w}} = 0$ for an arbitrary $\mathfrak{w}$, and therefore $\bar{\nabla} = \nabla'$.

We show now that the curvature of the crystal connection $\bar{\nabla}$ vanishes (Noll 1967), i.e. it satisfies the relation

$$\bar{\mathfrak{r}}(\mathfrak{w}_1, \mathfrak{w}_2, \mathfrak{w}_3) = \bar{\nabla}_{\mathfrak{w}_1}\bar{\nabla}_{\mathfrak{w}_2}\mathfrak{w}_3 - \bar{\nabla}_{\mathfrak{w}_2}\bar{\nabla}_{\mathfrak{w}_1}\mathfrak{w}_3 - \bar{\nabla}_{[\mathfrak{w}_1,\mathfrak{w}_2]}\mathfrak{w}_3 = 0. \tag{4.2}$$

Indeed, let $\mathbf{c}$ be an arbitrary constant vector field on $\mathcal{B}$. Since $\bar{\nabla}$ is the crystal connection we have $\bar{\nabla}_{\mathfrak{w}_1}\mathbf{c} = \mathbf{0}$ for all $\mathfrak{w}_1 \in T\mathcal{B}$. Hence, the definition (3.7) shows that $\mathfrak{r}(\mathfrak{w}_1, \mathfrak{w}_2, \mathbf{c}) = 0$ for all $\mathfrak{w}_1, \mathfrak{w}_2 \in T\mathcal{B}$. From this it is easy to see that the equation (4.2) must hold. It has to be emphasized that in our continuum model we are dealing only with translational dislocations. In a more general framework incorporating also disclinations the curvature need not be zero (see Anthony 1970; Maugin 1993).

Of special interest in finite elastoplasticity with microstructure is the Cartan torsion of the crystal connection

$$\bar{\mathfrak{t}}(\mathfrak{w}_1, \mathfrak{w}_2) = \bar{\nabla}_{\mathfrak{w}_1}\mathfrak{w}_2 - \bar{\nabla}_{\mathfrak{w}_2}\mathfrak{w}_1 - [\mathfrak{w}_1, \mathfrak{w}_2]. \tag{4.3}$$

Let us derive now spatial representations of the crystal connection (4.1) and of the Cartan torsion (4.3) relative to the different references. Substituting (2.4) into (4.1) we can express the covariant derivative (4.1) in the form

$$\bar{\nabla}_{\mathfrak{w}_1}\mathfrak{w}_2 = \mathbb{K}_0^{-1}[D\mathbf{W}_2 + \mathbf{F}^{p-1}(D\mathbf{F}^p)\mathbf{W}_2]\mathbf{W}_1, \tag{4.4}$$

where $\mathbf{W}_1 = \mathbb{K}_0 \mathfrak{w}_1, \mathbf{W}_2 = \mathbb{K}_0 \mathfrak{w}_2$, and D denotes the derivative relative to $\mathbb{K}_0$, $D = d_{\mathbb{K}_0}$. The expression in the square brackets represents a (1,1) tensor field on $\mathcal{V}$ and can be written in components as follows

$$(\mathbf{W}_2)^A_{|B} = (\mathbf{W}_2)^A_{,B} + \Gamma^A_{BC}(\mathbf{W}_2)^C, \tag{4.5}$$

where

$$\Gamma^A_{BC} = (\mathbf{F}^{p-1})^A_\alpha (\mathbf{F}^p)^\alpha_{C,B}. \tag{4.6}$$

Here the comma preceding indices is used to denote the partial derivative with respect to the corresponding co-ordinate [3]. According to (4.5) and (4.6), Γ^A_{BC} can be called the Christoffel symbols of the crystal connection relative to the initial reference. With the formula for the Lie bracket

$$[\mathfrak{w}_1, \mathfrak{w}_2] = \mathbb{K}_0^{-1}[(D\mathbf{W}_2)\mathbf{W}_1 - (D\mathbf{W}_1)\mathbf{W}_2]$$

and with (4.4) the torsion tensor (4.3) can be written as

$$\bar{\mathbf{t}}(\mathfrak{w}_1, \mathfrak{w}_2) = \mathbb{K}_0^{-1}[\mathbf{T}^p(\mathbf{W}_1, \mathbf{W}_2)],$$

$$\mathbf{T}^p(\mathbf{W}_1, \mathbf{W}_2) = \mathbf{F}^{p-1}[((D\mathbf{F}^p)\mathbf{W}_2)\mathbf{W}_1 - ((D\mathbf{F}^p)\mathbf{W}_1)\mathbf{W}_2], \tag{4.7}$$

or in components

$$(\mathbf{T}^p)^A_{BC} = \Gamma^A_{BC} - \Gamma^A_{CB} = (\mathbf{F}^{p-1})^A_\alpha[(\mathbf{F}^p)^\alpha_{C,B} - (\mathbf{F}^p)^\alpha_{B,C}]. \tag{4.8}$$

It is easy to see that $\mathbf{T}^p$ is skew-symmetric with respect to the covariant indices. It is obtained as the push-forward of $\bar{\mathbf{t}}$ to the initial configuration.

Similarly, with (2.3) the same covariant derivative (4.1) on $\mathcal{B}$ can also be represented in the form

$$\bar{\nabla}_{\mathfrak{w}_1}\mathfrak{w}_2 = \mathbb{K}_t^{-1}[d\mathbf{w}_2 + \mathbf{F}^e(d\mathbf{F}^{e-1})\mathbf{w}_2]\mathbf{w}_1, \tag{4.9}$$

with $\mathbf{w}_1 = \mathbb{K}_t \mathfrak{w}_1, \mathbf{w}_2 = \mathbb{K}_t \mathfrak{w}_2$, and d denoting the derivative relative to $\mathbb{K}_t$, $d = d_{\mathbb{K}_t}$. In component form the expression in brackets in (4.9) can be written as follows

$$(\mathbf{w}_2)^a_{|b} = (\mathbf{w}_2)^a_{,b} + \gamma^a_{bc}(\mathbf{w}_2)^c, \tag{4.10}$$

with the Christoffel symbols defined by

$$\gamma^a_{bc} = (\mathbf{F}^e)^a_\alpha (\mathbf{F}^{e-1})^\alpha_{c,b}. \tag{4.11}$$

[3] We refer upper case indices to coordinates in $\mathcal{B}_0$, lower case indices to coordinates in $\mathcal{B}_t$, and Greek indices to the anholonomic basis introduced by $\bar{\mathbb{K}}_t$.

Consequently, the torsion tensor (4.3) has the following representation relative to the current description

$$\bar{\mathbf{t}}(\mathbf{w}_1, \mathbf{w}_2) = \mathbb{K}_t^{-1}[\mathbf{t}^e(\mathbf{w}_1, \mathbf{w}_2)],$$

$$\mathbf{t}^e(\mathbf{w}_1, \mathbf{w}_2) = \mathbf{F}^e[((d\mathbf{F}^{e-1})\mathbf{w}_2)\mathbf{w}_1 - ((d\mathbf{F}^{e-1})\mathbf{w}_1)\mathbf{w}_2], \tag{4.12}$$

or in components

$$(\mathbf{t}^e)^a_{bc} = \gamma^a_{bc} - \gamma^a_{cb} = (\mathbf{F}^e)^a_\alpha[(\mathbf{F}^{e-1})^\alpha_{c,b} - (\mathbf{F}^{e-1})^\alpha_{b,c}]. \tag{4.13}$$

Thus, the tensor $\mathbf{t}^e$ can be intepreted as the push-forward of $\bar{\mathbf{t}}$ to the current configuration (Bilby *et al* 1955).

Substituting $\mathbf{W}_1 = \mathbf{F}^{p-1}\bar{\mathbf{w}}_1, \mathbf{W}_2 = \mathbf{F}^{p-1}\bar{\mathbf{w}}_2$ into (4.7) and using the definition (3.2) we can represent the torsion tensor $\bar{\mathbf{t}}$ relative to the anholonomic crystal reference as follows

$$\bar{\mathbf{t}}(\mathbf{w}_1, \mathbf{w}_2) = \bar{\mathbb{K}}_t^{-1}[\bar{\mathbf{t}}^p(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2)],$$

$$\bar{\mathbf{t}}^p(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2) = \mathbf{F}^p[((\bar{d}\,\mathbf{F}^{p-1})\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2 - ((\bar{d}\,\mathbf{F}^{p-1})\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1], \tag{4.14}$$

$$(\bar{\mathbf{t}}^p)^\alpha_{\beta\gamma} = (\mathbf{F}^p)^\alpha_A[(\mathbf{F}^{p-1})^A_{\beta,\gamma} - (\mathbf{F}^{p-1})^A_{\gamma,\beta}].$$

In a similar way, from (4.12) we have

$$\bar{\mathbf{t}}(\mathbf{w}_1, \mathbf{w}_2) = \bar{\mathbb{K}}_t^{-1}[\bar{\mathbf{t}}^e(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2)],$$

$$\bar{\mathbf{t}}^e(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2) = \mathbf{F}^{e-1}[((\bar{d}\,\mathbf{F}^e)\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2 - ((\bar{d}\,\mathbf{F}^e)\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1], \tag{4.15}$$

$$(\bar{\mathbf{t}}^e)^\alpha_{\beta\gamma} = (\mathbf{F}^{e-1})^\alpha_a[(\mathbf{F}^e)^a_{\beta,\gamma} - (\mathbf{F}^e)^a_{\gamma,\beta}],$$

with $\bar{\mathbf{w}}_1 = \bar{\mathbb{K}}_t\mathbf{w}_1, \bar{\mathbf{w}}_2 = \bar{\mathbb{K}}_t\mathbf{w}_2$, and $\bar{d}$ denoting the derivative relative to $\bar{\mathbb{K}}_t$ (in components it is denoted by the comma preceding Greek indices). We shall ascribe to $\bar{\mathbf{t}} = \bar{\mathbf{t}}^e = \bar{\mathbf{t}}^p$ the physical meaning of the dislocation density, which is not a given characteristics of the material, but should be defined by the internal dynamics of the plastic flow (cf. Noll 1967; Wang 1967). From (4.7), (4.12),(4.14),(4.15) the following relations can be derived

$$\bar{\mathbf{t}}^p(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2) = \mathbf{F}^p\mathbf{T}^p(\mathbf{W}_1, \mathbf{W}_2),$$

$$(\bar{\mathbf{t}}^p)^\alpha_{\beta\gamma} = (\mathbf{F}^p)^\alpha_A(\mathbf{T}^p)^A_{BC}(\mathbf{F}^{p-1})^B_\beta(\mathbf{F}^{p-1})^C_\gamma, \tag{4.16}$$

$$\bar{\mathbf{t}}^c(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2) = \mathbf{F}^{e-1}\mathbf{t}^e(\mathbf{w}_1, \mathbf{w}_2),$$

$$(\bar{\mathbf{t}}^e)^\alpha_{\beta\gamma} = (\mathbf{F}^{e-1})^\alpha_a(\mathbf{t}^e)^a_{bc}(\mathbf{F}^e)^b_\beta(\mathbf{F}^e)^c_\gamma. \tag{4.17}$$

We see that $\bar{\mathbf{t}}$ is the push-forward (by $\mathbf{F}^p$) of $\mathbf{T}^p$ and the pull-back (by $\mathbf{F}^e$) of $\mathbf{t}^e$.

Let us consider the geometric interpretation of the tensor $\mathbf{t}^e$ (Bilby *et al* 1955, Kröner 1960). Take the closed contour $c(s)$ in the current configuration and consider the integral

$$(\bar{\mathbf{b}})^\alpha = -\oint_c (\mathbf{F}^{e-1})^\alpha_b \, dx^b. \tag{4.18}$$

If this integral would vanish for all closed contours, (4.18) would mean the compatibility of the elastic deformation. But as it was mentioned in Section 2, it is not so, in general, and this integral measures the degree of incompatibility of the elastic deformation. One can show that (4.18) coincides with Burger's vector in the limiting case of continuum model (if we let the lattice constant approach zero). The microscopic picture would look like Fig.3.

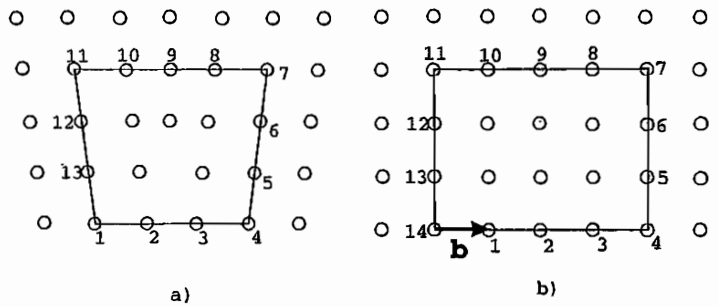

Figure 1.3: Definition of Burger's vector. a)current configuration; b)crystal reference.

Now let us apply Stokes' theorem to the contour integral (4.18)

$$(\bar{\mathbf{b}})^\alpha = \frac{1}{2}\int_A [(\mathbf{F}^{e-1})^\alpha_{c,b} - (\mathbf{F}^{e-1})^\alpha_{b,c}] \, dx^b \wedge dx^c, \tag{4.19}$$

where A denotes a surface with boundary c and $dx^b \wedge dx^c$ the oriented surface element. For infinitesimal contours c we get from (4.19)

$$(\bar{\mathbf{b}})^\alpha = \frac{1}{2}[(\mathbf{F}^{e-1})^\alpha_{c,b} - (\mathbf{F}^{e-1})^\alpha_{b,c}] \, dx^b \wedge dx^c. \tag{4.20}$$

Pushing Burger's vector forward to the current configuration gives

$$(\mathbf{b})^a = \frac{1}{2}(\mathbf{F}^e)^a_\alpha[(\mathbf{F}^{e-1})^\alpha_{c,b} - (\mathbf{F}^{e-1})^\alpha_{b,c}]\, dx^b \wedge dx^c$$

$$= \frac{1}{2}(\mathbf{t}^e)^a_{bc}\, dx^b \wedge dx^c. \tag{4.21}$$

This result provides the precise geometric interpretation of the dislocation density tensor.

1.5 Riemannian structures, strain measures and contortion

We define inner products and metrics on $\mathcal{T}$ induced by the following three references: $\mathbb{K}_0 = d\phi_0, \mathbb{K}_t = d\phi_t$, and $\bar{\mathbb{K}}_t$ as follows

$$\begin{aligned}
\mathfrak{G}(\mathfrak{w}_1, \mathfrak{w}_2) &= \mathbf{g}(\mathbb{K}_0\mathfrak{w}_1, \mathbb{K}_0\mathfrak{w}_2), \qquad & \mathfrak{G} &= \mathbb{K}_0^T\mathbf{g}\mathbb{K}_0, \\
\mathfrak{g}(\mathfrak{w}_1, \mathfrak{w}_2) &= \mathbf{g}(\mathbb{K}_t\mathfrak{w}_1, \mathbb{K}_t\mathfrak{w}_2), \qquad & \mathfrak{g} &= \mathbb{K}_t^T\mathbf{g}\mathbb{K}_t, \\
\bar{\mathfrak{g}}(\mathfrak{w}_1, \mathfrak{w}_2) &= \mathbf{g}(\bar{\mathbb{K}}_t\mathfrak{w}_1, \bar{\mathbb{K}}_t\mathfrak{w}_2), \qquad & \bar{\mathfrak{g}} &= \bar{\mathbb{K}}_t^T\mathbf{g}\bar{\mathbb{K}}_t.
\end{aligned} \tag{5.1}$$

These metric tensors define three Riemannian structures on $\mathcal{B}$ relative to the above mentioned references. One can say that $\mathfrak{G}$, $\mathfrak{g}$, and $\bar{\mathfrak{g}}$ are obtained from the metric $\mathbf{g}$ on $\mathcal{V}$ by using pull-back operations with $\mathbb{K}_0, \mathbb{K}_t$, and $\bar{\mathbb{K}}_t$, respectively (see Abraham, Marsden & Ratiu 1983; Marsden & Hughes 1983). From (5.1) it follows that

$$\mathfrak{g} = \mathbb{K}_0^T\mathbf{C}\mathbb{K}_0, \qquad \mathbf{C} = \mathbf{F}^T\mathbf{g}\mathbf{F}, \tag{5.2}$$

with $\mathbf{C}$ being the right Cauchy-Green deformation tensor. Analogously, we can prove that

$$\begin{aligned}
\mathfrak{G} &= \mathbb{K}_t^T\mathbf{c}\mathbb{K}_t, \qquad & \mathbf{c} &= \mathbf{F}^{-T}\mathbf{g}\mathbf{F}^{-1}, \\
\mathfrak{G} &= \bar{\mathbb{K}}_t^T\bar{\mathbf{c}}^p\bar{\mathbb{K}}_t, \qquad & \bar{\mathbf{c}}^p &= \mathbf{F}^{p-T}\mathbf{g}\mathbf{F}^{p-1}, \\
\mathfrak{g} &= \bar{\mathbb{K}}_t^T\bar{\mathbf{c}}^e\bar{\mathbb{K}}_t, \qquad & \bar{\mathbf{c}}^e &= \mathbf{F}^{eT}\mathbf{g}\mathbf{F}^e.
\end{aligned} \tag{5.3}$$

By using pull-back and push-forward operations we can also obtain the following elastic and plastic deformation tensors

$$\bar{\mathfrak{g}} = \mathbb{K}_0^T\mathbf{C}^p\mathbb{K}_0, \qquad \mathbf{C}^p = \mathbf{F}^{pT}\mathbf{g}\mathbf{F}^p, \tag{5.4}$$

$$\bar{\mathfrak{g}} = \mathbb{K}_t^T \mathbf{c}^e \mathbb{K}_t, \qquad \mathbf{c}^e = \mathbf{F}^{e-T} \mathbf{g} \mathbf{F}^{e-1}. \tag{5.5}$$

The formulae (5.2)-(5.5) give representations of different metrics relative to the initial and current description. From (5.2) and (5.3) we have

$$\bar{\mathbf{c}}^e = \mathbf{F}^{p-T} \mathbf{C} \mathbf{F}^{p-1}, \tag{5.6}$$

or in components

$$(\bar{\mathbf{c}}^e)_{\alpha\beta} = (\mathbf{C})_{AB} (\mathbf{F}^{p-1})^A_\alpha (\mathbf{F}^{p-1})^B_\beta. \tag{5.7}$$

One can also define uniquely torsion-free connections ∇°, ∇, and ∇^* associated with the respective metric tensors $\mathfrak{G}, \mathfrak{g}$, and $\bar{\mathfrak{g}}$ whose parallel translations preserve inner products (the fundamental theorem of Riemannian geometry). It is easy to show that the curvatures of ∇° and ∇ vanish (due to the compatibility of the total deformation), while the curvature of ∇^* in general does not (see Noll 1967).

To find the relation between $\bar{\nabla}$ and ∇^*, let us consider the expression

$$\bar{\mathfrak{d}}_{\mathfrak{w}} = \bar{\nabla}_{\mathfrak{w}} - \nabla^*_{\mathfrak{w}} = \bar{\mathfrak{d}} \mathfrak{w}. \tag{5.8}$$

The (1,2)-tensor field $\bar{\mathfrak{d}}$ is called the contortion of the crystal reference $\bar{\mathbb{K}}_t$. In the initial description it has the following components

$$D^A_{BC} = \Gamma^A_{BC} - \left\{ {A \atop BC} \right\}, \tag{5.9}$$

where $\left\{ {A \atop BC} \right\}$ are the Christoffel symbols of the Riemannian connection

$$\left\{ {A \atop BC} \right\} = \frac{1}{2} (\mathbf{C}^{p-1})^{AD} \left[(\mathbf{C}^p)_{BD,C} + (\mathbf{C}^p)_{CD,B} - (\mathbf{C}^p)_{BC,D} \right]. \tag{5.10}$$

It is easy to see that $\left\{ {A \atop BC} \right\}$ are symmetric with respect to the covariant indices, so that the Riemannian connection is torsion-free. The equation (5.8) written relative to the current description yields

$$d^a_{bc} = \gamma^a_{bc} - \left\{ {a \atop bc} \right\}, \tag{5.11}$$

with

$$\left\{ {a \atop bc} \right\} = \frac{1}{2} (\mathbf{c}^{e-1})^{ad} \left[(\mathbf{c}^e)_{bd,c} + (\mathbf{c}^e)_{cd,b} - (\mathbf{c}^e)_{bc,d} \right]. \tag{5.12}$$

Using the properties of the crystal reference $\bar{\mathbb{K}}_t$ one can show that (see Noll 1967)

$$2\bar{\mathfrak{g}}(\mathfrak{w}_1, (\bar{\mathfrak{d}} \mathfrak{w}_3) \mathfrak{w}_2) = \bar{\mathfrak{g}}(\mathfrak{w}_3, (\bar{t} \mathfrak{w}_1) \mathfrak{w}_2)$$

$$-\bar{\mathbf{g}}(\mathbf{w}_1, (\bar{\mathbf{t}}\mathbf{w}_2)\mathbf{w}_3) - \bar{\mathbf{g}}(\mathbf{w}_2, (\bar{\mathbf{t}}\mathbf{w}_3)\mathbf{w}_1). \tag{5.13}$$

Relative to the initial description it is equivalent to

$$2(\mathbf{C}^p)_{AB}D^B_{CD} = (\mathbf{C}^p)_{AB}(\mathbf{T}^p)^B_{CD} - (\mathbf{C}^p)_{CB}(\mathbf{T}^p)^B_{DA} - (\mathbf{C}^p)_{DB}(\mathbf{T}^p)^B_{AC}. \tag{5.14}$$

Similarly, relative to the current description we have

$$2(\mathbf{c}^e)_{ab}d^b_{cd} = (\mathbf{c}^e)_{ab}(\mathbf{t}^e)^b_{cd} - (\mathbf{c}^e)_{cb}(\mathbf{t}^e)^b_{da} - (\mathbf{c}^e)_{db}(\mathbf{t}^e)^b_{ac}. \tag{5.15}$$

According to the formula (5.14) contortion and torsion determine one another. It is also worth noting that $\bar{\nabla}\bar{\mathbf{g}} = \mathbf{0}$, and consequently the index raising and lowering operations with $\bar{\mathbf{g}}$ can be interchanged with the covariant derivative $\bar{\nabla}$.

1.6 Velocity and relative rates

The velocity and acceleration of the material point X at time t are the following spatial vectors

$$\dot{\mathbf{x}} = \frac{\partial}{\partial t}\phi(X,t), \tag{6.1}$$

$$\ddot{\mathbf{x}} = \frac{\partial}{\partial t}\dot{\mathbf{x}} = \frac{\partial^2}{\partial t^2}\phi(X,t). \tag{6.2}$$

Here and in what follows the dot is used to denote the partial time derivative with X kept fixed. Assuming the motion to be regular, we can express X as $X = \phi_t^{-1}(x)$ and substitute it into the equations (6.1),(6.2) to get the velocity and acceleration in the current description

$$\mathbf{v}(x,t) = \dot{\mathbf{x}}(\phi_t^{-1}(x), t), \tag{6.3}$$

$$\mathbf{a}(x,t) = \ddot{\mathbf{x}}(\phi_t^{-1}(x), t). \tag{6.4}$$

The following relation between $\mathbf{a}$ and $\mathbf{v}$ holds

$$\mathbf{a} = \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \mathrm{grad}\mathbf{v}. \tag{6.5}$$

We assume the existence of a mass form $d\mathfrak{m}$ on $T\mathcal{B}$. The mass of a submanifold $\mathcal{U}$ of $\mathcal{B}$ is defined as $\mathfrak{m}(\mathcal{U}) = \int_{\mathcal{U}} d\mathfrak{m}$. We can pull back the volume form dv on $\mathcal{V}$ by $\mathbb{K}_0, \mathbb{K}_t$, and $\bar{\mathbb{K}}_t$ to obtain the respective volume

forms $d\mathfrak{v}_0, d\mathfrak{v}$ and $d\bar{\mathfrak{v}}$ on $T\mathcal{B}$. We define mass densities $\mathfrak{r}_0, \mathfrak{r}$, and $\bar{\mathfrak{r}}$ relative to the respective references $\mathbb{K}_0, \mathbb{K}_t$, and $\bar{\mathbb{K}}_t$ as follow

$$\mathfrak{r}_0 d\mathfrak{v}_0 = \mathfrak{r} d\mathfrak{v} = \bar{\mathfrak{r}} d\bar{\mathfrak{v}} = d\mathfrak{m} \quad \text{(conservation of mass)}. \tag{6.6}$$

From these definitions and from (2.2)-(2.4) it follows at once that

$$\mathfrak{r}_0 = \mathfrak{r} J = \bar{\mathfrak{r}} J^p. \tag{6.7}$$

Denoting $\rho(x,t) = \mathfrak{r}(X,t)$ and taking the partial time derivative of the first equation in (6.7) we get the conservation of mass in the current description

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\rho\mathbf{v} = 0. \tag{6.7}$$

Let us consider now the rates of deformation and dislocation density. If some tensor is given on the body manifold $\mathcal{B}$, one can easily define its rate by taking the material time derivative (the partial time derivative with X kept fixed). Examples of such rates are the following tensors

$$\dot{\mathbf{g}} = \frac{\partial}{\partial t}\mathbf{g}(X,t)\mid_{X=\text{const}} = 2\mathbb{K}_t^T \mathbf{d}\mathbb{K}_t, \qquad \mathbf{d} = \frac{1}{2}(\mathbf{l}^T\mathbf{g} + \mathbf{g}\mathbf{l}), \tag{6.8}$$

$$\dot{\bar{\mathbf{g}}} = \frac{\partial}{\partial t}\bar{\mathbf{g}}(X,t)\mid_{X=\text{const}} = 2\bar{\mathbb{K}}_t^T \bar{\mathbf{d}}^p \bar{\mathbb{K}}_t, \qquad \bar{\mathbf{d}}^p = \frac{1}{2}(\bar{\mathbf{l}}^{pT}\mathbf{g} + \mathbf{g}\bar{\mathbf{l}}^p), \tag{6.9}$$

$$\dot{\mathbf{t}}(\mathfrak{w}_1, \mathfrak{w}_2) = \bar{\mathbb{K}}_t^{-1} 2\bar{\mathbf{z}}(\bar{\mathfrak{w}}_1, \bar{\mathfrak{w}}_2), \quad \bar{\mathfrak{w}}_1 = \bar{\mathbb{K}}_t \mathfrak{w}_1, \quad \bar{\mathfrak{w}}_2 = \bar{\mathbb{K}}_t \mathfrak{w}_2, \tag{6.10}$$

$$2\bar{\mathbf{z}}(\bar{\mathfrak{w}}_1, \bar{\mathfrak{w}}_2) = [((d\bar{\mathbf{l}}^p)\bar{\mathfrak{w}}_2)\bar{\mathfrak{w}}_1 - ((d\bar{\mathbf{l}}^p)\bar{\mathfrak{w}}_1)\bar{\mathfrak{w}}_2], \tag{6.11}$$

with $\mathbf{l} = \dot{\mathbf{F}}\mathbf{F}^{-1}, \bar{\mathbf{l}}^p = \dot{\mathbf{F}}^p\mathbf{F}^{p-1}$, the tensors $\mathbf{d}$ and $\bar{\mathbf{d}}^p$ denoting the total and plastic deformation rates, respectively, and the tensor $\bar{\mathbf{z}}$ to be called the dislocation drift rate.

This definition leads naturally to the so-called time derivative relative to the reference $\mathbb{K}$ for spatial tensors, calculated by pulling them back to the body manifold by $\mathbb{K}$, taking the partial time derivative with X kept fixed and pushing the result forward to the spatial configuration by the same $\mathbb{K}$. We shall denote this derivative by $\mathfrak{L}_{\mathbb{K}}$. It is easy to prove that

$$\mathfrak{L}_{\mathbb{K}_t}\mathbf{t} = \mathfrak{L}_{\mathbf{v}}\mathbf{t} \tag{6.12}$$

for every spatial tensor $\mathbf{t}$, with $\mathfrak{L}_{\mathbf{v}}$ denoting the Lie derivative with respect to the velocity field $\mathbf{v}$. Note that the relative time derivative of scalar functions coincide with their material time derivative

$$\mathfrak{L}_{\mathbb{K}_t} f = \frac{\partial f}{\partial t} + \mathbf{v}\cdot d_{\mathbb{K}_t} f = D_t f.$$

Directly from the definition of the time derivative relative to the reference $\mathbb{K}$ and from (5.5)-(5.7),(4.11) it can be proved that

$$\mathfrak{L}_{\mathbb{K}_t}\mathbf{c} = 0, \qquad \frac{1}{2}\mathfrak{L}_{\mathbb{K}_t}\mathbf{g} = \mathbf{d}, \qquad \frac{1}{2}\mathfrak{L}_{\mathbb{K}_t}\mathbf{c}^e = \mathbf{d}^p, \tag{6.13}$$

$$\mathfrak{L}_{\bar{\mathbb{K}}_t}\bar{\mathbf{c}}^p = 0, \qquad \frac{1}{2}\mathfrak{L}_{\bar{\mathbb{K}}_t}\mathbf{g} = \bar{\mathbf{d}}^p, \qquad \frac{1}{2}\mathfrak{L}_{\bar{\mathbb{K}}_t}\bar{\mathbf{c}}^e = \bar{\mathbf{d}}, \tag{6.14}$$

$$\frac{1}{2}\mathfrak{L}_{\bar{\mathbb{K}}_t}\bar{\mathbf{t}} = \bar{\mathbf{z}}, \qquad \frac{1}{2}\mathfrak{L}_{\mathbb{K}_t}\mathbf{t}^e = \mathbf{z}, \tag{6.15}$$

$$\mathbf{z}(\mathbf{w}_1, \mathbf{w}_2) = \frac{1}{2}\mathbf{F}^e[((d\bar{\mathbf{l}}^p)\mathbf{F}^{e-1}\mathbf{w}_2)\mathbf{w}_1 - ((d\bar{\mathbf{l}}^p)\mathbf{F}^{e-1}\mathbf{w}_1)\mathbf{w}_2], \tag{6.16}$$

with $\mathbf{d}^p = \mathbf{F}^{e-T}\bar{\mathbf{d}}^p\mathbf{F}^{e-1}, \bar{\mathbf{d}} = \mathbf{F}^{eT}\mathbf{d}\mathbf{F}^e$. The tensor $\mathbf{z}$ is called the (spatial) dislocation drift rate. The properties (6.13)-(6.16) will play an essential role in the subsequent study of the constitutive equations.

Chapter 2

Determination of the crystal reference

2.1 Differential equations for the inverse elastic deformation.

From the first chapter we have seen that the basic kinematic quantities such as the metric (strain) and the torsion (dislocation density) are defined through the crystal reference. Now let us consider the inverse problem of determining the crystal reference from its metric and torsion considered as the given tensor fields. Relative to the current description the problem can be formulated as follows: determine $\mathbf{F}^{e-1}$ from given $\mathbf{c}^e$ and $\mathbf{t}^e$, provided the current configuration is known. There are six independent components of the symmetric tensor $\mathbf{c}^e$ and nine independent components of the skew-symmetric tensor $\mathbf{t}^e$, from which nine components of the tensor $\mathbf{F}^{e-1}$ should be determined. It is clear that some constraints should be imposed on the problem to make it well-posed.

To solve this problem, let us derive the differential equation for $\mathbf{F}^{e-1}$. Taking the derivative of $\mathbf{F}^{e-1}$ relative to $\mathbb{K}_t$ we have

$$d\mathbf{F}^{e-1} = \mathbf{F}^{e-1}\boldsymbol{\gamma}, \tag{1.1}$$

or in commponents,

$$(\mathbf{F}^{e-1})^{\alpha}_{b,c} = (\mathbf{F}^{e-1})^{\alpha}_{a}\gamma^{a}_{cb}. \tag{1.2}$$

In the subsequence we will work out some formulae explicitly in commponents. According to (1.4.11), γ^a_{bc} are the Christoffel symbols of the crystal connection relative to the current reference. Since $\mathbf{c}^e$ and $\mathbf{t}^e$ are supposed to be given, γ^a_{be} can be expressed through $(\mathbf{c}^e)_{ab}$ and $(\mathbf{t}^e)^a_{bc}$ with the help of (1.5.11) and (1.5.15) according to

$$\gamma^a_{bc} = \left\{{a \atop be}\right\} + d^a_{bc}$$

$$= \frac{1}{2}(\mathbf{c}^{e-1})^{ad}\left[(\mathbf{c}^e)_{bd,c} + (\mathbf{c}^e)_{cd,b} - (\mathbf{c}^e)_{bc,d}\right]$$

$$+\frac{1}{2}\left[(\mathbf{t}^e)^a_{bc} - (\mathbf{c}^e)_{bd}(\mathbf{t}^e)^d_{cc}(\mathbf{c}^{e-1})^{ea} - (\mathbf{c}^e)_{cd}(\mathbf{t}^e)^d_{be}(\mathbf{c}^{e-1})^{ea}\right]. \qquad (1.3)$$

Eqn. (1.2) can then be considered as a system of partial differential equations for the nine components of $\mathbf{F}^{e-1}$. The existence of the solution of (1.2) is ensured if the following integrability conditions are fulfilled

$$(\mathbf{F}^{e-1})^\alpha_{b,dc} - (\mathbf{F}^{e-1})^\alpha_{b,cd} = 0. \qquad (1.4)$$

Let us calculate the second derivative of $\mathbf{F}^{e-1}$ taking (1.2) into account to obtain

$$(\mathbf{F}^{e-1})^\alpha_{b,dc} = (\mathbf{F}^{e-1})^\alpha_a\left[\gamma^a_{ci}\gamma^i_{db} + \gamma^a_{db,c}\right]. \qquad (1.5)$$

Therefore, the integrability conditions (1.4) can be rewritten in the form

$$(\mathbf{F}^{e-1})^\alpha_a r^a_{bcd} = 0, \qquad (1.6)$$

with

$$r^a_{bcd} = \gamma^a_{ci}\gamma^i_{db} - \gamma^a_{di}\gamma^i_{cb} + \gamma^a_{db,c} - \gamma^a_{cb,d}. \qquad (1.7)$$

Eqn. (1.7) expresses nothing else but the component representation of the curvature tensor $\bar{\mathbf{r}}$ of (1.4.2) relative to the current reference (cf. any standard texbook on differential geometry, e.g. Sternberg 1983). Thus, the integrability conditions (1.6) require the curvature tensor (1.7) to vanish.

If the integrability conditions (1.6) are fulfilled, one can integrate Eqn. (1.2) to determine $\mathbf{F}^{e-1}$. Let us fix some arbitrary point X_0 of the body. Let $c(s)$ be a curve connecting X_0 with another arbitrary point X such that $c(0) = X_0$. Relative to the current description this curve is described by the equations

$$x^a = x^a(s), \quad x^a(0) = x^a_0. \qquad (1.8)$$

Multiplying both sides of Eqn. (1.2) by the tangent vector x'^c of the curve (the prime denotes here the derivative with respect to s) we get

$$\frac{d}{ds}\mathbf{F}^{e-1} = \mathbf{F}^{e-1}\mathbf{p}, \qquad (1.9)$$

with the tensor $\mathbf{p}$ having the components

$$p^a_b = \gamma^a_{cb}x'^c. \qquad (1.10)$$

Thus, the system of partial differential equations for $\mathbf{F}^{e-1}$ is transformed into the linear ordinary differential equation for $\mathbf{F}^{e-1}$ along the curve $c(s)$ with the tensor $\mathbf{p}$ as given function of s. Additionally, the following initial condition for $\mathbf{F}^{e-1}$ at $s = 0$ (at the point X_0) should be prescribed

$$\mathbf{F}^{e-1}(X_0) = \mathbf{F}_0^{e-1}. \tag{1.11}$$

Since the left stretch tensor $\mathbf{v}^e$ following from the polar decomposition theorem applied to $\mathbf{F}^e$ can be calculated from the metric $\mathbf{c}^e$, only three components of the rotation tensor should be prescribed at this point. The solution of (1.9), (1.11) has the form (see Gantmacher 1960)

$$\mathbf{F}^{e-1} = \mathbf{F}_0^{e-1}\boldsymbol{\omega}_s, \tag{1.12}$$

where $\boldsymbol{\omega}_s$ is the matricant of (1.9) defined by the tensor series

$$\boldsymbol{\omega}_s = \mathbf{i} + \int_0^s \mathbf{p}(\tau)\,d\tau + \int_0^s \left[\int_0^\tau \mathbf{p}(\tau_1)\,d\tau_1\right] \mathbf{p}(\tau)\,d\tau + \dots \tag{1.13}$$

Here $\mathbf{i}$ denotes the identity tensor. Due to the integrability conditions (1.4) the solution $\mathbf{F}^{e-1}$ does not depend on the choice of the curve $c(s)$. Therefore, if the body is simply connected the solution presented by (1.12)-(1.13) is unique. Eqs. (1.12), (1.13) valid for the nonlinear dislocation theory are analogous to those of Cesàro (1906) for the displacement field in linear elasticity and of Pietraszkiewicz (1982) and Pietraszkiewicz & Badur (1983) in nonlinear elasticity.

2.2 Differential equations for the inverse elastic rotation.

To determine the inverse elastic rotation let us consider the left polar decomposition

$$\mathbf{F}^e = \mathbf{v}^e\mathbf{R}^e, \quad \mathbf{F}^{e-1} = \mathbf{R}^{e-1}\mathbf{v}^{e-1}, \tag{2.1}$$

with $\mathbf{R}^e$ being the proper orthogonal elastic rotation tensor and $\mathbf{v}^e$ the left elastic stretch tensor. The equation $(2.1)_2$ in components take the form

$$(\mathbf{F}^{e-1})_b^a = (\mathbf{R}^{e-1})_a^\alpha (\mathbf{v}^{e-1})_b^a. \tag{2.2}$$

Since the stretch tensor $\mathbf{v}^{e-1}$ can be determined from $\mathbf{c}^e$ with the help of linear algebra, the problem of determining $\mathbf{F}^{e-1}$ from $\mathbf{c}^e$ and $\mathbf{t}^e$ reduces to

that of determining $\mathbf{R}^{e-1}$ from those two tensor fields. We derive now the corresponding differential equation. Taking the derivative of both sides of (2.2) we obtain

$$(\mathbf{F}^{e-1})^{\alpha}_{b,c} = (\mathbf{R}^{e-1})^{\alpha}_{a,c}(\mathbf{v}^{e-1})^{a}_{b} + (\mathbf{R}^{e-1})^{\alpha}_{a}(\mathbf{v}^{e-1})^{a}_{b,c}. \tag{2.3}$$

Substituting (2.3) into (1.2) we get

$$(\mathbf{R}^{e-1})^{\alpha}_{b,c} = (\mathbf{R}^{e-1})^{\alpha}_{a}\lambda^{a}_{eb}, \tag{2.4}$$

with

$$\lambda^{a}_{eb} = \left[(\mathbf{v}^{e-1})^{a}_{e}\gamma^{e}_{cd} - (\mathbf{v}^{e-1})^{a}_{d,e}\right](\mathbf{v}^{e})^{d}_{b}. \tag{2.5}$$

Since $\mathbf{v}^{e-1}$ and γ^{a}_{bc} can be expressed through the tensor fields $\mathbf{c}^{e}$ and $\mathbf{t}^{e}$ (cf. (1.3)) we can refer to (2.4) as the system of partial differential equations for $\mathbf{R}^{e-1}$ with the coefficients λ^{a}_{bc} considered as the known functions of X. Note that due to the proper orthogonality of $\mathbf{R}^{e-1}$ these coefficients λ^{a}_{bc} must be skew-symmetric with respect to the covariant indices.

The integrability conditions for (2.4) read

$$(\mathbf{R}^{e-1})^{\alpha}_{b,dc} - (\mathbf{R}^{e-1})^{\alpha}_{b,cd} = 0. \tag{2.6}$$

Performing analogous transformations as in Section 1 we can rewrite (2.6) in the form

$$(\mathbf{R}^{e-1})^{\alpha}_{a}k^{a}_{bcd} = 0, \tag{2.7}$$

with

$$k^{a}_{bdc} = \lambda^{a}_{ce}\lambda^{e}_{db} - \lambda^{a}_{de}\lambda^{e}_{cb} + \lambda^{a}_{db,c} - \lambda^{a}_{eb,d}. \tag{2.8}$$

Thus, the integrability conditions (2.6) require the tensor k^{a}_{bcd} of (2.8) to vanish. To show the equivalence of (2.7) and (1.6) let us establish the relationship between the curvature tensor r^{a}_{bcd} and the tensor k^{a}_{bed}. Using the definition (2.5) of λ^{a}_{bc} to express γ^{a}_{bc} in terms of λ^{a}_{bc} and $(\mathbf{v}^{e-1})^{a}_{b}$, and substituting them into the expression (1.7) we can prove that

$$r^{a}_{bcd} = (\mathbf{v}^{e-1})^{a}_{c}(\mathbf{v}^{e})^{f}_{b}k^{e}_{fcd}. \tag{2.9}$$

Since $\mathbf{v}^{e}$ is positive definite, the curvature tensor r^{a}_{bcd} vanishes if and only if the tensor k^{a}_{bcd} vanishes. Thus, the equivalence of (2.7) and (1.6) is proved.

If the integrability conditions (2.7) are fulfilled, one can integrate Eqs. (2.4) in a manner similar to that in Section 1. Let $c(s)$ be the curve

connecting X_0 with another arbitrary point X. Multiplying both sides of Eqs. (2.4) with the tangent vector x'^c of the curve we get

$$\frac{d}{ds}\mathbf{R}^{e-1} = \mathbf{R}^{e-1}\mathbf{q}, \tag{2.10}$$

with

$$q^a_b = \lambda^a_{cb}x'^c. \tag{2.11}$$

The solution of (2.10) has the form

$$\mathbf{R}^{e-1} = \mathbf{R}^{e-1}_0 \boldsymbol{\upsilon}_s, \tag{2.12}$$

where $\boldsymbol{\upsilon}_s$ is the matricant of (2.10) defined by the series

$$\boldsymbol{\upsilon}_s = \mathbf{i} + \int_0^s \mathbf{q}(\tau)\,d\tau + \int_0^s \left[\int_0^\tau \mathbf{q}(\tau_1)\,d\tau_1\right] \mathbf{q}(\tau)\,d\tau + \ldots \tag{2.13}$$

2.3 Dual problems for the plastic deformation and plastic rotation.

Since $\mathbf{C}^p$ and $\mathbf{T}^p$ are dual representations of the metric and torsion with respect to the initial description, the dual problem of determining $\mathbf{F}^p$ and $\mathbf{R}^p$ from the given $\mathbf{C}^p$ and $\mathbf{T}^p$ can be solved in a similar manner. Not going into details we simply enumerate formulae without proof.

The system of partial differential equations for $\mathbf{F}^p$ reads

$$(\mathbf{F}^p)^\alpha_{B,C} = (\mathbf{F}^p)^\alpha_A \Gamma^A_{CB}, \tag{3.1}$$

where Γ^A_{BC} are the Christoffel symbols of the crystal connection relative to the initial reference. Since $\mathbf{C}^p$ and $\mathbf{T}^p$ are assumed to be given, Γ^A_{BC} can be expressed through them with the help of (1.5.9) and (1.5.14). Namely,

$$\begin{aligned}\Gamma^A_{BC} &= \left\{{A \atop BC}\right\} + D^A_{BC} \\ &= \frac{1}{2}(\mathbf{C}^{p-1})^{AD}\left[(\mathbf{C}^p)_{BD,C} + (\mathbf{C}^p)_{CD,B} - (\mathbf{C}^p)_{BC,D}\right] \\ &\quad + \frac{1}{2}\left[(\mathbf{T}^p)^A_{BC} - (\mathbf{C}^p)_{BD}(\mathbf{T}^p)^D_{CE}(\mathbf{C}^{p-1})^{EA}\right. \\ &\quad \left. -(\mathbf{C}^p)_{CD}(\mathbf{T}^p)^D_{BE}(\mathbf{C}^{p-1})^{EA}\right].\end{aligned} \tag{3.2}$$

The integrability conditions for (3.1) are

$$(\mathbf{F}^p)^\alpha_A R^A_{BCD} = 0, \tag{3.3}$$

with

$$R^A_{BCD} = \Gamma^A_{CE}\Gamma^E_{DB} - \Gamma^A_{DE}\Gamma^E_{CB} + \Gamma^A_{DB,C} - \Gamma^A_{CB,D}. \tag{3.4}$$

Eq. (3.4) expresses nothing else but the component representation of the curvature tensor $\bar{\mathbf{r}}$ of (1.4.2) relative to the initial reference.

If the conditions (3.3) are fulfilled, the solution of (3.1) can be given in the form

$$\mathbf{F}^p = \mathbf{F}^p_0 \boldsymbol{\Omega}_s, \tag{3.5}$$

with $\mathbf{F}^p_0$ denoting the prescribed value of $\mathbf{F}^p$ at the point X_0 and $\boldsymbol{\Omega}_s$ defined by the following matricant

$$\boldsymbol{\Omega}_s = \mathbf{i} + \int_0^s \mathbf{P}(\tau)\, d\tau + \int_0^s \left[\int_0^\tau \mathbf{P}(\tau_1)\, d\tau_1\right] \mathbf{P}(\tau)\, d\tau + \ldots. \tag{3.6}$$

The tensor $\mathbf{P}$ in (3.6) has the components

$$P^A_B = \Gamma^a_{CB} X'^C, \tag{3.7}$$

with X'^C the tangent vector of the curve $c(s)$ in the initial description. Due to the integrability conditions (3.3) the solution $\mathbf{F}^p$ does not depend on the choice of the curve $c(s)$. Therefore if the body is simply connected the solution presented by (3.5)-(3.6) is unique.

To determine the plastic rotation let us consider the right polar decomposition

$$\mathbf{F}^p = \mathbf{R}^p \mathbf{U}^p, \tag{3.8}$$

with $\mathbf{R}^p$ denoting the proper orthogonal plastic rotation tensor and $\mathbf{U}^p$ the plastic stretch tensor. The equation (3.8) in component form reads

$$(\mathbf{F}^p)^\alpha_B = (\mathbf{R}^p)^\alpha_A (\mathbf{U}^p)^A_B. \tag{3.9}$$

The differential equation for $\mathbf{R}^p$ is given by

$$(\mathbf{R}^p)^\alpha_{B,C} = (\mathbf{R}^p)^\alpha_A \Lambda^A_{CB}, \tag{3.10}$$

with

$$\Lambda^A_{CB} = \left[(\mathbf{U}^p)^A_E \Gamma^E_{CD} - (\mathbf{U}^p)^A_{D,C}\right] (\mathbf{U}^{p-1})^D_B. \tag{3.11}$$

The integrability condition for (3.10) requires that

$$(\mathbf{R}^p)^{\alpha}_{A} K^{A}_{BCD} = 0, \tag{3.12}$$

where

$$K^{A}_{BDC} = \Lambda^{A}_{CE}\Lambda^{E}_{DB} - \Lambda^{A}_{DE}\Lambda^{E}_{CB} + \Lambda^{A}_{DB,C} - \Lambda^{A}_{CB,D}. \tag{3.13}$$

It can be checked that

$$R^{A}_{BCD} = (\mathbf{U}^p)^{A}_{E}(\mathbf{U}^{p-1})^{F}_{B} K^{E}_{FCD}. \tag{3.14}$$

The analogous formula in nonlinear elasticity derived by Shield (1973) contains a printing error. Because $\mathbf{U}^p$ is positive definite the curvature tensor R^{A}_{BCD} vanishes if and only if the tensor K^{A}_{BCD} vanishes. Thus, the equivalence between (3.3) and (3.12) is proved.

If the integrability conditions (3.12) are fulfilled, one can integrate Eqs. (3.10) in the same manner as before. The solution of (3.10) has the form

$$\mathbf{R}^p = \mathbf{R}^p_0 \boldsymbol{\Upsilon}_s, \tag{3.15}$$

where $\boldsymbol{\Upsilon}_s$ is the matricant of (3.10) defined by the series

$$\boldsymbol{\Upsilon}_s = \mathbf{i} + \int_0^s \mathbf{Q}(\tau)\, d\tau + \int_0^s \left[\int_0^{\tau} \mathbf{Q}(\tau_1)\, d\tau_1\right] \mathbf{Q}(\tau)\, d\tau + \ldots. \tag{3.16}$$

The tensor $\mathbf{Q}$ in (3.16) is given by

$$Q^{A}_{B} = \Lambda^{A}_{CB} X'^{C}. \tag{3.17}$$

2.4 Linearization.

It is interesting to carry out the linearization of the equations derived in Chapters 1 and 2 in order to compare them with the well-known Kröner theory (Kröner 1958,1960). Let us assume that the deformation fields $\mathbf{F}, \mathbf{F}^p, \mathbf{F}^e$ have the following form

$$\begin{aligned} \mathbf{F} &= \mathbf{1} + \boldsymbol{\beta}, \\ \mathbf{F}^p &= \mathbf{1} + \boldsymbol{\beta}^p, \\ \mathbf{F}^e &= \mathbf{1} + \boldsymbol{\beta}^e, \end{aligned} \tag{4.1}$$

where $\boldsymbol{\beta}, \boldsymbol{\beta}^p, \boldsymbol{\beta}^e$ are small compared with $\mathbf{1}$. In this case the references $\mathbb{K}_0, \mathbb{K}_t$ and $\bar{\mathbb{K}}_t$ differ from each other by small distorsions, so that they can

be identified. Therefore, there is no need to distinguish between upper case, lower case and Greek indices. We also can choose the metric $\mathbf{g}$ to coincide with $\mathbf{1}$ and we can identify the tangent and cotangent spaces. Thus, there is no need to distinguish between co- and contravariant tensors. Substituting (4.1) into (1.2.5) and neglecting higher order terms we obtain the additive decomposition

$$\boldsymbol{\beta} = \boldsymbol{\beta}^e + \boldsymbol{\beta}^p. \tag{4.2}$$

As a consequence, the symmetric and skew-symmetric parts of $\boldsymbol{\beta}$ decompose also additively into

$$\boldsymbol{\epsilon} = \frac{1}{2}(\boldsymbol{\beta} + \boldsymbol{\beta}^T) = \boldsymbol{\epsilon}^e + \boldsymbol{\epsilon}^p, \tag{4.3}$$

$$\boldsymbol{\omega} = \frac{1}{2}(\boldsymbol{\omega} - \boldsymbol{\omega}^T) = \boldsymbol{\omega}^e + \boldsymbol{\omega}^p, \tag{4.4}$$

where $\boldsymbol{\epsilon}^e, \boldsymbol{\epsilon}^p$ and $\boldsymbol{\omega}^e, \boldsymbol{\omega}^p$ are the symmetric and skew-symmetric parts of $\boldsymbol{\beta}^e$ and $\boldsymbol{\beta}^p$, respectively. The metric tensors $\mathbf{C}^p$ and $\mathbf{c}^e$ are approximated by

$$\mathbf{C}^p = \mathbf{F}^{pT}\mathbf{F}^p \approx \mathbf{1} + 2\boldsymbol{\epsilon}^p, \tag{4.5}$$

$$\mathbf{c}^e = \mathbf{F}^{e-T}\mathbf{F}^{e-1} \approx \mathbf{1} - 2\boldsymbol{\epsilon}^e. \tag{4.6}$$

One can see that in the linearized theory it is more convenient to use the small strain tensors $\boldsymbol{\epsilon}^p$ and $\boldsymbol{\epsilon}^e$ instead of $\mathbf{C}^p$ and $\mathbf{c}^e$.

Let us consider now the dislocation density tensors $\mathbf{T}^p$ and $\mathbf{t}^e$. Linearizing (1.5.6) and (1.5.7) we get

$$(\mathbf{T}^p)_{abc} \approx (\boldsymbol{\beta}^p)_{ac,b} - (\boldsymbol{\beta}^p)_{ab,c}, \tag{4.7}$$

$$(\mathbf{t}^e)_{abc} \approx -[(\boldsymbol{\beta}^e)_{ac,b} - (\boldsymbol{\beta}^e)_{ab,c}]. \tag{4.8}$$

Subtracting (4.8) from (4.7) we obtain

$$(\mathbf{T}^p)_{abc} - (\mathbf{t}^e)_{abc} \approx (\boldsymbol{\beta})_{ac,b} - (\boldsymbol{\beta})_{ab,c}. \tag{4.9}$$

Since $\mathbf{T}^p$ is the "pull-back" of $\mathbf{t}^e$, in the linearized theory they become approximately equal. Relation (4.9) then reads

$$(\boldsymbol{\beta})_{ac,b} - (\boldsymbol{\beta})_{ab,c} = 0. \tag{4.10}$$

This simply means that the total distortion $\boldsymbol{\beta}$ must be compatible, or equivalently, there exists a displacement field $\mathbf{w}$ such that

$$(\boldsymbol{\beta})_{ab} = (\mathbf{w})_{a,b}. \tag{4.11}$$

As in the case of strain measures, in the linearized theory it is more convenient to use the second rank tensor $\boldsymbol{\alpha}$, which is related to $\mathbf{T}^p$ as follows

$$\alpha_{ab} = \frac{1}{2}\varepsilon_{bcd}(\mathbf{T}^p)_{acd}, \tag{4.12}$$

with ε_{abc} denoting the permutation symbols. Eqn. (4.7) in terms of $\boldsymbol{\alpha}$ takes the following classical form (Kröner, 1958)

$$\boldsymbol{\alpha} = \mathrm{curl}\boldsymbol{\beta}^p, \quad (\boldsymbol{\alpha} = \nabla \times \boldsymbol{\beta}^p). \tag{4.13}$$

The tensor $\boldsymbol{\alpha}$ is called the dislocation density tensor of the linearized theory. Eqn. (4.8) has the form

$$\mathrm{curl}\boldsymbol{\beta}^e = -\boldsymbol{\alpha}, \quad (\nabla \times \boldsymbol{\beta}^e = -\boldsymbol{\alpha}). \tag{4.14}$$

The differential equations for the inverse elastic deformation (1.1) after linearization takes the form

$$\begin{aligned} -(\boldsymbol{\beta}^e)_{ac,b} &= -[(\boldsymbol{\epsilon}^e)_{ba,c} + (\boldsymbol{\epsilon}^e)_{ca,b} - (\boldsymbol{\epsilon}^e)_{bc,a}] \\ &+\frac{1}{2}[(\mathbf{t}^e)_{abc} - (\mathbf{t}^e)_{bca} - (\mathbf{t}^e)_{cba}]. \end{aligned} \tag{4.15}$$

The linearized integrability conditions (1.6) reduce to

$$\begin{aligned} r_{abcd} &= [-(\boldsymbol{\epsilon}^e)_{da,bc} + (\boldsymbol{\epsilon}^e)_{db,ac} + (\boldsymbol{\epsilon}^e)_{ca,bd} - (\boldsymbol{\epsilon}^e)_{cb,ad}] \\ &+\frac{1}{2}[(\mathbf{t}^e)_{adb} - (\mathbf{t}^e)_{dba} - (\mathbf{t}^e)_{bda}]_{,c} \\ &-\frac{1}{2}[(\mathbf{t}^e)_{acb} - (\mathbf{t}^e)_{cba} - (\mathbf{t}^e)_{bca}]_{,d} = 0. \end{aligned} \tag{4.16}$$

Multiplying (4.16) by $\frac{1}{4}\varepsilon_{iab}\varepsilon_{jcd}$ and taking its symmetric and skew-symmetric parts, we reduce it to the following two conditions:

$$\alpha_{ij,j} = 0, \quad (\mathrm{div}\boldsymbol{\alpha} = 0), \tag{4.17}$$

and

$$\varepsilon_{iab}\varepsilon_{jcd}(\boldsymbol{\epsilon}^e)_{db,ac} + \frac{1}{2}(\varepsilon_{iab}\alpha_{bj,a} + \varepsilon_{jab}\alpha_{bi,a}) = 0,$$

or, in Kröner's notation,

$$\mathrm{inc}\boldsymbol{\epsilon}^e - (\boldsymbol{\alpha} \times \nabla)_{sym} = 0. \tag{4.18}$$

These equations were first obtained by Kröner (1958).

In a similar manner one can show that the linearized equation (2.4) for the elastic rotation tensor is equivalent to

$$\text{curl}\boldsymbol{\omega}^e = -\text{curl}\boldsymbol{\epsilon}^e - \boldsymbol{\alpha}. \tag{4.19}$$

It is easy to see that the linearized equations for the plastic deformation and plastic rotation are equivalent to (4.15) and (4.19). This kind of duality is due to the additive decomposition of the total compatible displacement gradient $\boldsymbol{\beta}$ according to (4.2).

Chapter 3

Statics

3.1 Free energy density and principle of frame indifference

Let us consider an elastoplastic body with continuously distributed dislocations under the condition of constant temperature. We postulate the existence of a free energy per unit crystal volume of such a body. Relative to the crystal reference, which is assumed at the moment to be given, this free energy is supposed to depend on the elastic deformation $\mathbf{F}^e$ as well as on its derivative $\bar{d}\mathbf{F}^e$,

$$\mathfrak{w} = \bar{\mathfrak{w}}(X, \mathbf{F}^e, \bar{d}\mathbf{F}^e). \tag{1.1}$$

The stress state arising within elastoplastic bodies is produced as a result of elastic deformation leading to the energy stored in these bodies. Therefore, if we superpose a rigid-body motion onto the actual motion of the body we must also expect the energy to remain unchanged. Such a scalar function is called frame indifferent.

Consider two motions $\phi(X,t)$ and $\phi^*(X,t)$ of a body. Neither of them will be assumed rigid in general. These motions are regarded as differing from one another by a rigid-body motion if at any instant they are related by

$$\phi^*(X,t) = c(t) + \mathbf{Q}(t)[\phi(X,t) - x_0], \tag{1.2}$$

where $c(t)$ is a time-dependent point, $\mathbf{Q}(t)$ is a time-dependent orthogonal tensor, and x_0 is a fixed point. A scalar function is said to be frame indifferent, if it does not change its value when a rigid-body motion (1.2) is superposed. Now we want to show that if the free energy density (1.1) is frame indifferent, it can depend only on $X, \bar{\mathbf{c}}^e$ and $\bar{\mathbf{t}}$.

First of all, when the rigid-body motion (1.2) is superposed, the current reference becomes

$$\mathbb{K}_t^* = \mathbf{Q}\mathbb{K}_t. \tag{1.3}$$

The crystal reference is assumed to be the same for both motions. Therefore, according to (1.2.3) the elastic deformation is transformed by the rule

$$\mathbf{F}^{e*} = \mathbf{Q}\mathbf{F}^e. \tag{1.4}$$

Since the derivative $\bar{d}$ is calculated with respect to the same crystal reference $\bar{\mathbb{K}}_t$, we have

$$\bar{d}\mathbf{F}^{e*} = \mathbf{Q}\bar{d}\mathbf{F}^e. \tag{1.5}$$

Using the definitions (1.4.15) and $(1.5.3)_3$ one can see that

$$\bar{\mathbf{c}}^{e*} = \mathbf{F}^{e*T}\mathbf{g}\mathbf{F}^{e*} = \mathbf{F}^{eT}\mathbf{Q}^T\mathbf{g}\mathbf{Q}\mathbf{F}^e = \bar{\mathbf{c}}^e \tag{1.6}$$

and

$$\begin{aligned}\bar{\mathbf{t}}^*(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2) &= \mathbf{F}^{e*-1}[((\bar{d}\mathbf{F}^{e*})\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1 - ((\bar{d}\mathbf{F}^{e*})\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2] \\ &= \mathbf{F}^{e-1}\mathbf{Q}^{-1}[((\mathbf{Q}\bar{d}\mathbf{F}^{e*})\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1 - ((\mathbf{Q}\bar{d}\mathbf{F}^{e*})\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2] = \bar{\mathbf{t}}(\bar{\mathbf{w}}_1, \bar{\mathbf{w}}_2)\end{aligned} \tag{1.7}$$

hold. Hence, any function depending on $X, \bar{\mathbf{c}}^e$ and $\bar{\mathbf{t}}^e$ is frame indifferent.

Now let us consider two motions $\phi(X,t)$ and $\phi^*(X,t)$ with the same elastic strain $\bar{\mathbf{c}}^e = \bar{\mathbf{c}}^{e*}$ and the same dislocation density $\bar{\mathbf{t}} = \bar{\mathbf{t}}^*$. We want to show that these motions differ from one another by a rigid-body motion. Let $\mathbb{K}_t$ and $\mathbb{K}_t^*$ be the current references of these motions, respectively, and let

$$\mathbb{K}_t^* = \mathbf{Q}(X,t)\mathbb{K}_t^*, \quad \mathbf{F}^{e*} = \mathbf{Q}(X,t)\mathbf{F}^e, \tag{1.8}$$

with $\mathbf{Q}(X,t)$ denoting a deformation field. We have to show that $\mathbf{Q}$ is orthogonal and depends only on t. In fact, from the condition $\bar{\mathbf{c}}^e = \bar{\mathbf{c}}^{e*}$ and (1.8) we have

$$\mathbf{F}^{e*T}\mathbf{g}\mathbf{F}^{e*} = \mathbf{F}^{eT}\mathbf{Q}^T(X,t)\mathbf{g}\mathbf{Q}(X,t)\mathbf{F}^e = \mathbf{F}^{eT}\mathbf{g}\mathbf{F}^e. \tag{1.9}$$

Hence, $\mathbf{Q}(X,t)$ satisfies the identity

$$\mathbf{Q}^T(X,t)\mathbf{g}\mathbf{Q}(X,t) = \mathbf{g}, \tag{1.10}$$

or, equivalently saying, $\mathbf{Q}(X,t)$ is orthogonal. Substituting $(1.8)_2$ into the definition (1.4.15) and using the identity $\bar{\mathbf{t}} = \bar{\mathbf{t}}^*$ we have

$$\mathbf{F}^{e*-1}[((\bar{d}\mathbf{F}^{e*})\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1 - ((\bar{d}\mathbf{F}^{e*})\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2]$$

$$= \mathbf{F}^{e-1}\mathbf{Q}^{-1}[((\mathbf{Q}\bar{d}\,\mathbf{F}^e)\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1 - ((\mathbf{Q}\bar{d}\,\mathbf{F}^e)\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2]$$
$$+\mathbf{F}^{e-1}\mathbf{Q}^{-1}[(\bar{d}\,\mathbf{Q}(\mathbf{F}^e\bar{\mathbf{w}}_2))\bar{\mathbf{w}}_1 - (\bar{d}\,\mathbf{Q}(\mathbf{F}^e\bar{\mathbf{w}}_1))\bar{\mathbf{w}}_2]$$
$$= \mathbf{F}^{e-1}[((\bar{d}\,\mathbf{F}^e)\bar{\mathbf{w}}_2)\bar{\mathbf{w}}_1 - ((\bar{d}\,\mathbf{F}^e)\bar{\mathbf{w}}_1)\bar{\mathbf{w}}_2]. \tag{1.11}$$

From (1.11) follows the identity

$$\mathbf{F}^{e-1}\mathbf{Q}^{-1}[(\bar{d}\,\mathbf{Q}(\mathbf{F}^e\bar{\mathbf{w}}_2))\bar{\mathbf{w}}_1 - (\bar{d}\,\mathbf{Q}(\mathbf{F}^e\bar{\mathbf{w}}_1))\bar{\mathbf{w}}_2] = 0. \tag{1.12}$$

Replacing the derivative $\bar{d}$ in (1.12) by d according to (1.3.2), we can show that

$$\mathbf{Q}^{-1}[((d\mathbf{Q})\mathbf{w}_2)\mathbf{w}_1 - ((d\mathbf{Q})\mathbf{w}_1)\mathbf{w}_2] = 0. \tag{1.13}$$

Eqs. (1.10) and (1.13) lead to the problem of determining the deformation field $\mathbf{Q}$, when its metric is $\mathbf{g}$ and its torsion vanishes (cf. with the problem of determining $\mathbf{F}^p$ from $\mathbf{C}^p$ and $\mathbf{T}^p$ in Section 2.3). It is easy to see that the Christoffel symbols associated with $\mathbf{Q}$ are equal to zero, and the equation for $\mathbf{Q}$ reads

$$d\mathbf{Q} = 0. \tag{1.14}$$

The solution of (1.14) is $\mathbf{Q} = \mathbf{Q}_0(t)$ ($\mathbf{Q}$ does not depend on X). Thus, according to the principle of frame indifference the energy of these motions should be the same and we can write

$$\mathfrak{w} = \hat{\mathfrak{w}}(X, \bar{\mathbf{c}}^e, \bar{\mathbf{t}}). \tag{1.15}$$

This result is in agreement with Kröner's requirement stating that the free energy density can depend only on the elastic strain and on the dislocation density (Kröner 1992).

It is also worth noting the difference between (1.15) and the formula for the free energy density in the model of defective crystals proposed by Davini (1986). Davini's approach is not based on the multiplicative decomposition of the total deformation into elastic and plastic parts. Additionally, it excludes the total deformation from the constitutive list. The free energy in Davini's theory depends on the metric induced by the lattice vector fields (directors) and on the measures of defects (dislocation and vacancy densities). Since the inelastic deformations can change the directors, and therefore the metric tensor, it follows that the free energy density in Davini's theory does not depend on the metric induced by the

elastic deformation and on the dislocation density *alone*. This seems to be in conflict with the above mentioned Kröner's requirement.

When the plastic deformation is absent so that $\mathbf{F}^p = \mathbf{1}$, and $\mathbf{F}^e = \mathbf{F}$ is compatible, then $\bar{\mathbf{c}}^e = \mathbf{C}$, and $\bar{\mathbf{t}} = \mathbf{0}$. The formula (1.15) reduces in this case to the classical one for hyperelastic bodies

$$W = W(X, \mathbf{C}). \tag{1.16}$$

Since $\bar{\mathbf{c}}^e$ and $\bar{\mathbf{t}}$ are the pull-backs of the metric $\mathbf{g}$ and the torsion $\mathbf{t}^e$, respectively, we can regard them as functions of the point values of $\mathbf{F}^e, \mathbf{g}$, and $\mathbf{t}^e$ (cf. with formulae (1.4.18) and (1.5.3)). Therefore, $\bar{\mathfrak{w}}$ becomes a function of $X, \mathbf{F}^e, \mathbf{g}$, and $\mathbf{t}^e$. We can say that relative to the current reference $\mathbb{K}_t$ the free energy per unit volume of the current configuration takes the form

$$w = J^{e-1}\hat{\mathfrak{w}}(X, \bar{\mathbf{c}}^e(\mathbf{F}^e, \mathbf{g}), \bar{\mathbf{t}}(\mathbf{F}^e, \mathbf{t}^e)) = \hat{w}(X, \mathbf{F}^e, \mathbf{g}, \mathbf{t}^e), \tag{1.17}$$

where

$$J^{e-1} = \det \mathbf{F}^{e-1}. \tag{1.18}$$

Note that $\mathbf{t}^e$ is an objective third rank tensor, which under the superposed rigid-body motion is transformed according to

$$\mathbf{t}^{e*}(\mathbf{w}_1^*, \mathbf{w}_2^*) = \mathbf{Q}\mathbf{t}^e(\mathbf{w}_1, \mathbf{w}_2),$$

where $\mathbf{w}_1^* = \mathbf{Q}\mathbf{w}_1, \mathbf{w}_2^* = \mathbf{Q}\mathbf{w}_2$. The function $\hat{w}$ may, in general, depend on $\mathbf{F}^e$ explicitly. Only in special cases (isotropic materials, for instance) $\hat{w}$ depends on $\mathbf{F}^e$ through $\mathbf{c}^e$. Under the superposed rigid-body motion the energy density $\hat{w}$ must be frame indifferent, so that

$$\hat{w}(X, \mathbf{Q}\mathbf{F}^e, \mathbf{g}, \mathbf{t}^{e*}) = \hat{w}(X, \mathbf{F}^e, \mathbf{g}, \mathbf{t}^e). \tag{1.19}$$

Analogously, when referred to the initial description $\mathbb{K}_0$ the free energy per unit volume of the initial configuration takes the form

$$W = J^p\hat{\mathfrak{w}}(X, \bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \bar{\mathbf{t}}(\mathbf{F}^p, \mathbf{T}^p)) = \hat{W}(X, \mathbf{F}^p, \mathbf{C}, \mathbf{T}^p), \tag{1.20}$$

with

$$J^p = \det \mathbf{F}^p, \tag{1.21}$$

in full agreement with the covariance principle. Thus, we can see the duality and the equivalence between the initial and current descriptions (see e.g.

Green & Naghdi 1965; Sedov 1965; Lee 1969; Le & Stumpf 1993*a*). If the body is made of the same material at all points then W does not depend on X explicitly, so that

$$W = J^p \hat{\mathfrak{w}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \bar{\mathbf{t}}(\mathbf{F}^p, \mathbf{T}^p)) = \hat{W}(\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p). \tag{1.22}$$

For simplicity we shall further consider only homogeneous materials whose free energy is given by (1.22).

The formula (1.1) satisfies still another important criterium. The free energy of an elastoplastic body per unit crystal volume defined in this way depends only on the current and relaxed states, and it is insensitive to the change of the initial reference. This means that if we superpose an arbitrary initial deformation on the initial reference and keep the crystal and current references fixed, the energy $\hat{\mathfrak{w}}$ will remain unchanged. We shall call this property the principle of initial scaling indifference.

Let $\mathbf{X}$ be the position vector of an arbitrary point X in a chosen coordinate system. The superposed initial deformation transform $\mathbf{X}$ into the new position $\mathbf{X}^*$ given by

$$\mathbf{X}^* = \boldsymbol{\Phi}(\mathbf{X}). \tag{1.23}$$

Under (1.23) the initial reference will change according to

$$\mathbb{K}_0^* = \mathbf{F}_0 \mathbb{K}_0, \tag{1.24}$$

where $\mathbf{F}_0$ is the following initial deformation

$$\mathbf{F}_0 = D\boldsymbol{\Phi}. \tag{1.25}$$

Since the crystal and current references remain the same, the formulae (1.1.2)-(1.1.4) yield the following transformation rules

$$\mathbf{F}^* = \mathbf{F}\mathbf{F}_0^{-1}, \quad \mathbf{F}^{p*} = \mathbf{F}^p\mathbf{F}_0^{-1}, \quad \mathbf{F}^{e*} = \mathbf{F}^e. \tag{1.26}$$

For simplicity, we show the transformation rule for $D\mathbf{F}^p$ directly in components

$$(D\mathbf{F}^p)^{*\alpha}_{BC} = \frac{\partial((\mathbf{F}^p)^\alpha_D(\mathbf{F}_0^{-1})^D_B)}{\partial X^{*C}} = \frac{\partial((\mathbf{F}^p)^\alpha_D(\mathbf{F}_0^{-1})^D_B)}{\partial X^E}(\mathbf{F}_0^{-1})^E_C$$

$$= (\mathbf{F}^p)^\alpha_{D,E}(\mathbf{F}_0^{-1})^D_B(\mathbf{F}_0^{-1})^E_C + (\mathbf{F}^p)^\alpha_D\frac{\partial(\mathbf{F}_0^{-1})^D_B}{\partial X^E}(\mathbf{F}_0^{-1})^E_C. \tag{1.27}$$

According to the principle of initial scaling indifference the free energy density per unit crystal volume $\hat{\mathfrak{w}}(\bar{\mathbf{c}}^e, \bar{\mathbf{t}})$ should remain unchanged under the transformations (1.23), (1.26) and (1.27). The group of transformations associated with (1.23) will be called the rescaling group. Thus, up to the factor J^p, the energy (1.22) is invariant with respect to the rescaling group (1.23). This has far reaching consequences, which will be discussed later.

3.2 Principle of virtual work

Let $\mathbb{K}_0$ be chosen as the fixed reference, and let $\mathbf{X}$ and $\mathbf{x}$ be position vectors of the point X in the initial and current configuration, respectively. Then it is immediate that $\mathbf{F} = D\mathbf{x}$. Now the energy of an arbitrary sub-body $\mathcal{U}$ can be expressed in the form

$$I = \int_{\mathcal{U}_0} W(\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p)\, dv, \tag{2.1}$$

with $\mathcal{U}_0 = \phi_0(\mathcal{U})$, W denoting the free energy density relative to the initial reference, which is, in general, a function of $\mathbf{F}, \mathbf{F}^p$ and $D\mathbf{F}^p$. We shall first analyze the general situation, postponing the consideration of the energy density given by (1.22) for later.

Let us consider now a one-parameter family of configurations $\mathbf{x}(\mathbf{X}, \epsilon)$ and plastic deformations $\mathbf{F}^p(\mathbf{X}, \epsilon)$. We define a virtual displacement $(\delta\mathbf{x}, \delta\mathbf{F}^p)$ as follows

$$(\delta\mathbf{x}, \delta\mathbf{F}^p) = (\frac{\partial \mathbf{x}}{\partial \epsilon} \mid_{\epsilon=0}, \frac{\partial \mathbf{F}^p}{\partial \epsilon} \mid_{\epsilon=0}). \tag{2.2}$$

Assuming the external macro- and microforce to be zero, we postulate the following principle of virtual work

$$\delta I = \int_{\partial \mathcal{U}_0} (\mathbf{P}_\nu \cdot \delta\mathbf{x} + < \mathbf{P}^d_\nu, \delta\mathbf{F}^p >)\, da \tag{2.3}$$

to hold for an arbitrary sub-body $\mathcal{U}$, with $\mathbf{P}_\nu$ denoting the macrotraction, $\mathbf{P}^d_\nu$ the microtraction [1] (the small index d of this (1,1)-tensor indicates the

[1] The prescription of the microtraction on the boundary means that we are on the next to Cauchy's level of detailed description of the continuum (the level of Mikrostrukturmechanik, in Kröner's terminology, Kröner 1992). Therefore one should not treate $\mathbf{F}^p$ as the internal variable in Kestin's sense (cf. Kestin 1987), but should rather consider it as the microscopical degrees of freedom which can be measured and controlled in principle. Of course, the method of practical measurement of the microtraction is still far from being settled, and this is a field of future work for experimentists.

action on dislocations), da the area form in $\mathcal{V}$. Here the variation of I is defined as follows

$$\delta I = \frac{d}{d\epsilon} I[\mathbf{x}(\mathbf{X},\epsilon), \mathbf{F}^p(\mathbf{X},\epsilon)] \mid_{\epsilon=0} . \tag{2.4}$$

A somewhat different point of view on admissible variations and thermodynamics when dislocations and plasticity are concerned is discussed by Ericksen (1983).

We calculate now the variation of I (see e.g. Berdichevsky 1983)

$$\delta I = \int_{\mathcal{U}_0} \left(\left\langle \frac{\partial W}{\partial \mathbf{F}}, \delta \mathbf{F} \right\rangle + \left\langle \frac{\partial W}{\partial \mathbf{F}^p}, \delta \mathbf{F}^p \right\rangle + \left\langle \frac{\partial W}{\partial D\mathbf{F}^p}, \delta D\mathbf{F}^p \right\rangle \right) dv. \tag{2.5}$$

Introducing the relations $\delta \mathbf{F} = D\delta\mathbf{x}$ and $\delta D\mathbf{F}^p = D\delta\mathbf{F}^p$ into (2.5) and integrating it by parts we obtain

$$\begin{aligned} \delta I = \int_{\mathcal{U}_0} \left(-\left\langle \mathrm{Div}\frac{\partial W}{\partial \mathbf{F}}, \delta\mathbf{x} \right\rangle + \left\langle \frac{\partial W}{\partial \mathbf{F}^p}, \delta\mathbf{F}^p \right\rangle - \left\langle \mathrm{Div}\frac{\partial W}{\partial D\mathbf{F}^p}, \delta\mathbf{F}^p \right\rangle \right) dv \\ + \int_{\partial\mathcal{U}_0} \left(\left\langle \frac{\partial W}{\partial \mathbf{F}}\mathbf{N}, \delta\mathbf{x} \right\rangle + \left\langle \frac{\partial W}{\partial D\mathbf{F}^p}\mathbf{N}, \delta\mathbf{F}^p \right\rangle \right) da, \end{aligned} \tag{2.6}$$

where $\mathbf{N}$ is the outer normal to $\partial\mathcal{U}_0$, the boundary of $\mathcal{U}_0$. Substituting (2.6) into (2.3), one arrives at the following equilibrium equations

$$\mathrm{Div}\mathbf{P} = \mathbf{0}, \qquad \mathbf{P} = \mathbf{g}^{-1}\frac{\partial W}{\partial \mathbf{F}}, \tag{2.7}$$

$$\mathrm{Div}\mathbf{P}^d - \mathbf{J} = \mathbf{0}, \qquad \mathbf{P}^d = \frac{\partial W}{\partial D\mathbf{F}^p}, \tag{2.8}$$

with Div denoting the divergence operator associated with D, and $\mathbf{J}$ defined by

$$\mathbf{J} = \frac{\partial W}{\partial \mathbf{F}^p}. \tag{2.9}$$

We call $\mathbf{P}$ the (first Piola-Kirchhoff) macrostress tensor, $\mathbf{P}^d$ the microstress (2,1)-tensor (contravariant of rank 2 and covariant of rank 1, with components $(\mathbf{P}^d)^{AB}_{\alpha}$), and $\mathbf{J}$ the internal microforce ((1,1)-tensor). The boundary conditions for $\mathbf{P}$ and $\mathbf{P}^d$ are

$$\mathbf{P}\mathbf{N} = \mathbf{P}_\nu, \tag{2.10}$$

$$\mathbf{P}^d\mathbf{N} = \mathbf{P}^d_\nu. \tag{2.11}$$

Let us calculate $\mathbf{P}, \mathbf{P}^d, \mathbf{J}$ using the stored energy density given by (1.22). It can be directly seen that

$$\mathbf{P} = \mathbf{F}\mathbf{S}, \qquad \mathbf{S} = 2\frac{\partial \hat{W}}{\partial \mathbf{C}} = J^p \mathbf{F}^{p-1} \bar{\mathbf{s}} \mathbf{F}^{p-T}, \tag{2.12}$$

$$\bar{\mathbf{s}} = 2\frac{\partial \hat{\mathfrak{w}}}{\partial \bar{\mathbf{c}}^e}, \tag{2.13}$$

$$\mathbf{P}^d = -\mathbf{F}^{p-T}\mathbf{S}^d, \qquad \mathbf{S}^d = 2\frac{\partial \hat{W}}{\partial \mathbf{T}^p}, \tag{2.14}$$

$$\mathbf{S}^d(\mathbf{W}) = J^p \mathbf{F}^{p-1} \bar{\mathbf{s}}^d(\bar{\mathbf{w}}) \mathbf{F}^{p-T}, \tag{2.15}$$

$$\bar{\mathbf{s}}^d = 2\frac{\partial \hat{\mathfrak{w}}}{\partial \bar{\mathbf{t}}}. \tag{2.16}$$

The tensor $\mathbf{S}$ is symmetric and corresponds to the second Piola-Kirchhoff stress tensor in elasticity and elastoplasticity. The (2,1)-tensor $\mathbf{S}^d$ is skew-symmetric with respect to its contravariant components, and can be called the microcouple with reference to $\mathbb{K}_0$. We demonstrate the calculation of $\mathbf{J}$ in components using (2.9) and (1.22)

$$(\mathbf{J})_\alpha^A = \left.\frac{\partial W}{\partial (\mathbf{F}^p)_A^\alpha}\right|_{\mathbf{F}, D\mathbf{F}^p} = \frac{\partial J^p}{\partial (\mathbf{F}^p)_A^\alpha}\hat{\mathfrak{w}} + J^p \frac{\partial \hat{\mathfrak{w}}}{\partial (\bar{\mathbf{c}}^e)_{\gamma\delta}} \left.\frac{\partial (\bar{\mathbf{c}}^e)_{\gamma\delta}}{\partial (\mathbf{F}^p)_A^\alpha}\right|_{\mathbf{F}}$$

$$+ J^p \frac{\partial \hat{\mathfrak{w}}}{\partial (\bar{\mathbf{t}})_{\gamma\delta}^\beta} \left.\frac{\partial (\bar{\mathbf{t}})_{\gamma\delta}^\beta}{\partial (\mathbf{F}^p)_A^\alpha}\right|_{D\mathbf{F}^p}. \tag{2.17}$$

First of all, from the definition of determinant it is easy to show that

$$\frac{\partial J^p}{\partial (\mathbf{F}^p)_A^\alpha} = J^p (\mathbf{F}^{p-1})_\alpha^A. \tag{2.18}$$

Let us calculate now the second term in (2.17). Differentiating (1.5.7) we have

$$\left.\frac{\partial (\bar{\mathbf{c}}^e)_{\gamma\delta}}{\partial (\mathbf{F}^p)_A^\alpha}\right|_{\mathbf{F}} = \frac{\partial (\mathbf{F}^{p-1})_\gamma^C}{\partial (\mathbf{F}^p)_A^\alpha} (\mathbf{C})_{CD} (\mathbf{F}^{p-1})_\delta^D$$

$$+ (\mathbf{F}^{p-1})_\gamma^C (\mathbf{C})_{CD} \frac{\partial (\mathbf{F}^{p-1})_\delta^D}{\partial (\mathbf{F}^p)_A^\alpha}. \tag{2.19}$$

Using the identity $\mathbf{F}^{p-1}\mathbf{F}^p = \mathbf{1}$ one can show that

$$\frac{\partial (\mathbf{F}^{p-1})_\gamma^C}{\partial (\mathbf{F}^p)_A^\alpha} = -(\mathbf{F}^{p-1})_\alpha^C (\mathbf{F}^{p-1})_\gamma^A. \tag{2.20}$$

Substituting (2.19), and (2.20) into the second term of (2.17) and using the formula (2.12) we obtain

$$J^p \frac{\partial \hat{\mathfrak{w}}}{\partial (\bar{\mathbf{c}}^e)_{\gamma\delta}} \frac{\partial (\bar{\mathbf{c}}^e)_{\gamma\delta}}{\partial (\mathbf{F}^p)^{\alpha}_{A}}\bigg|_{\mathbf{F}} = -(\mathbf{F}^{p-1})^{C}_{\alpha}(\mathbf{C})_{CD}(\mathbf{S})^{DA}. \tag{2.21}$$

To calculate the last term in (2.17) we note that according to (1.4.7) and (1.4.16) (or (1.4.14))

$$(\bar{\mathbf{t}})^{\beta}_{\gamma\delta} = [(\mathbf{F}^p)^{\beta}_{D,C} - (\mathbf{F}^p)^{\beta}_{C,D}](\mathbf{F}^{p-1})^{C}_{\gamma}(\mathbf{F}^{p-1})^{D}_{\beta}. \tag{2.22}$$

Differentiating (2.22) in a similar manner as before, with the use of (2.20), we get

$$\frac{\partial (\bar{\mathbf{t}})^{\beta}_{\gamma\delta}}{\partial (\mathbf{F}^p)^{\alpha}_{A}}\bigg|_{D\mathbf{F}^p} = (\bar{\mathbf{t}})^{\beta}_{\gamma\alpha}(\mathbf{F}^{p-1})^{A}_{\delta} + (\bar{\mathbf{t}})^{\beta}_{\alpha\delta}(\mathbf{F}^{p-1})^{A}_{\gamma}. \tag{2.23}$$

Substituting this into the last term of (2.17) and recalling (2.15) and (2.16) we have

$$\begin{aligned} J^p \frac{\partial \hat{\mathfrak{w}}}{\partial (\bar{\mathbf{t}})^{\beta}_{\gamma\delta}} \frac{\partial (\bar{\mathbf{t}})^{\beta}_{\gamma\delta}}{\partial (\mathbf{F}^p)^{\alpha}_{A}}\bigg|_{D\mathbf{F}^p} &= (\bar{\mathbf{t}})^{\beta}_{\alpha\delta}(\bar{\mathbf{s}}^d)^{\gamma\delta}_{\beta}(\mathbf{F}^{p-1})^{A}_{\gamma} \\ &= (\mathbf{F}^{p-1})^{C}_{\alpha}(\mathbf{T}^p)^{B}_{CD}(\mathbf{S}^d)^{DA}_{B} \end{aligned} \tag{2.24}$$

Finally, combining (2.18), (2.21) and (2.24) we obtain

$$(\mathbf{J})^{A}_{\alpha} = (\mathbf{F}^{p-1})^{C}_{\alpha}\left[-(\mathbf{C})_{CD}(\mathbf{S})^{DA} + \hat{W}\delta^{A}_{C} + (\mathbf{T}^p)^{B}_{CD}(\mathbf{S}^d)^{DA}_{B}\right]. \tag{2.25}$$

Thus, the microforce is the pull-back (by one leg) to the crystal of the tensor in the square brackets, which, in turn, is the sum of Eshelby's tensor $-\mathbf{CS} + \hat{W}\mathbf{1}$ and of the tensor with components $(\mathbf{T}^p)^{B}_{CD}(\mathbf{S}^d)^{DA}_{B}$. The physical meaning of the former is to account for the action of the surrounding elastic field on dislocations (Eshelby 1951; Epstein & Maugin 1990), the latter tensor can be interpreted as representing the interaction between dislocations.

According to (2.14) the microstress tensor $\mathbf{P}^d$ is skew-symmetric with respect to the contravariant components. Therefore, applying the Div operator to (2.8) once more, one should get the identity

$$\mathrm{Div}\mathbf{J} = \mathbf{0}. \tag{2.26}$$

We check (2.26) directly in components. First, we rewrite (2.25) in terms of $\mathbf{P}$ and $\mathbf{P}^d$

$$(\mathbf{J})^A_\alpha = (\mathbf{F}^{p-1})^B_\alpha \left\{ W\delta^A_B - g_{ab}(\mathbf{P})^{aA}(\mathbf{F})^b_B \right.$$
$$\left. -(\mathbf{P}^d)^{CA}_\beta [(\mathbf{F}^p)^\beta_{C,B} - (\mathbf{F}^p)^\delta_{B,C}] \right\}. \tag{2.27}$$

Applying the Div operator to (2.27) we have

$$(\mathbf{J})^A_{\alpha,A} = (\mathbf{F}^{p-1})^B_{\alpha,A} \left\{ W\delta^A_B - g_{ab}(\mathbf{P})^{aA}(\mathbf{F})^b_B \right.$$
$$\left. -(\mathbf{P}^d)^{CA}_\beta [(\mathbf{F}^p)^\beta_{C,B} - (\mathbf{F}^p)^\delta_{B,C}] \right\}$$
$$+(\mathbf{F}^{p-1})^B_\alpha \left\{ W_{,B} - g_{ab}(\mathbf{P}^{aA}_{,A}(\mathbf{F})^b_B - g_{ab}(\mathbf{P})^{aA}(\mathbf{F})^b_{B,A} \right.$$
$$-(\mathbf{P}^d)^{CA}_{\beta,A} [(\mathbf{F}^p)^\beta_{C,B} - (\mathbf{F}^p)^\delta_{B,C}]$$
$$\left. -(\mathbf{P}^d)^{CA}_\beta [(\mathbf{F}^p)^\beta_{C,BA} - (\mathbf{F}^p)^\delta_{B,CA}] \right\}. \tag{2.28}$$

Using the identity $\mathbf{F}^{p-1}\mathbf{F}^p = \mathbf{1}$ one can derive the following formula

$$(\mathbf{F}^{p-1})^B_{\alpha,A} = -(\mathbf{F}^{p-1})^C_\alpha (\mathbf{F}^p)^\beta_{C,A} (\mathbf{F}^{p-1})^B_\beta. \tag{2.29}$$

Substituting (2.29) into (2.28) and taking (2.7) and (2.8) into account, one can see that the right-hand side of (2.28) vanishes. Note that in the case of nonvanishing body macroforce the microforce must also be assumed to be nonvanishing in order to keep the theory consistent. We restrict ourselves to the case of zero body force for simplicity.

3.3 Invariant properties and balance laws

In Section 1 the energy density of an elastoplastic body with dislocations is postulated to be frame indifferent with respect to the groups of translations and rotations of the Euclidean space $\mathcal{E}$. This means, under the superposed rigid-body motions

$$x^* = x + \mathbf{c} \tag{3.1}$$

and

$$x^* = x + \mathbf{Q}x \tag{3.2}$$

the energy functional (2.1) remains unchanged. Consequently, the variation of the energy δI vanishes for the following families of infinitesimal virtual displacements and plastic deformations

$$\delta\mathbf{x} = \mathbf{d}, \quad \delta\mathbf{F}^p = \mathbf{0}, \tag{3.3}$$

$$\delta \mathbf{x} = \boldsymbol{\omega}\mathbf{x}, \quad \delta \mathbf{F}^p = \mathbf{0}, \tag{3.4}$$

with $\mathbf{d} \in \mathcal{V}$ denoting an arbitrary constant vector, and $\boldsymbol{\omega}$ an arbitrary constant tensor satisfying the identity $(\mathbf{g}\boldsymbol{\omega})^T = -\mathbf{g}\boldsymbol{\omega}$ (infinitesimal generators of the transformations). Substituting (3.3) and (3.4) into the equation (2.3) and using the identity $\delta I = 0$ we arrive at the following balance equations for the stationary points

$$\int_{\partial \mathcal{U}_0} \mathbf{P}_\nu \, da = \mathbf{0}, \tag{3.5}$$

$$\int_{\partial \mathcal{U}_0} \mathbf{x} \times \mathbf{P}_\nu \, da = \mathbf{0}. \tag{3.6}$$

The equations (3.5) and (3.6) correspond to the balance of macromomentum and moment of macromomentum in integral form, respectively.

We derive now other balance equations associated with the invariant property of the energy density $\bar{\mathfrak{w}}$ (or W, up to the factor J^p) with repect to the rescaling group (1.23). Here and in what follows we shall work in components explicitly. Consider the following one-parameter family of homogeneous initial deformation

$$X^{*A} = (\mathbf{F}_0)^A_B X^B, \quad \mathbf{F}_0 = \text{ const.} \tag{3.7}$$

The homogeneous deformation $\mathbf{F}_0(\alpha)$ depends on the parameter α in such a way that $\mathbf{F}_0(0) = \mathbf{1}$. Hence, (3.7) is the subgroup of the rescaling group (1.23) and the transformation rules (1.26) and (1.27) hold. Since the free energy density $\hat{\mathfrak{w}}$ is initial scaling indifferent, we have the identity

$$W(\mathbf{F}^*, \mathbf{F}^{p*}, (D\mathbf{F}^p)^*) = \det \mathbf{F}^{p*} \, \hat{\mathfrak{w}}(\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p) \tag{3.8}$$

with $\mathbf{F}^*, \mathbf{F}^{p*}$ and $(D\mathbf{F}^p)^*$ given by (1.26) and (1.27). We differentiate (3.8) with respect to α at $\alpha = 0$, and use the rule of differentiation of composite functions and the following formulae

$$\begin{aligned}
\frac{d}{d\alpha}(\mathbf{F}^*)^a_A\Big|_{\alpha=0} &= (\mathbf{F})^a_B(\mathbf{G}_0)^B_A, \\
\frac{d}{d\alpha}(\mathbf{F}^{p*})^\alpha_A\Big|_{\alpha=0} &= (\mathbf{F}^p)^\alpha_B(\mathbf{G}_0)^B_A, \\
\frac{d}{d\alpha}(\mathbf{F}^p)^{*\alpha}_{B,C}\Big|_{\alpha=0} &= (\mathbf{F}^p)^\alpha_{D,C}(\mathbf{G}_0)^D_B + (\mathbf{F}^p)^\alpha_{B,D}(\mathbf{G}_0)^D_C,
\end{aligned} \tag{3.9}$$

where

$$\mathbf{G}_0 = \frac{d}{d\alpha}\mathbf{F}_0^{-1}\Big|_{\alpha=0}. \tag{3.10}$$

Taking into account (2.7), (2.8), (2.9) and (2.18) we get

$$g_{ab}(\mathbf{P})^{bA}(\mathbf{F})^a_B(\mathbf{G}_0)^B_A + (\mathbf{J})^{\cdot A}_{\alpha}(\mathbf{G}_0)^B_A$$
$$+(\mathbf{P}^d)^{BC}_{\alpha}\left[(\mathbf{F}^p)^{\alpha}_{D,C}(\mathbf{G}_0)^D_B + (\mathbf{F}^p)^{\alpha}_{B,D}(\mathbf{G}_0)^D_C\right] = W\delta^A_B(\mathbf{G}_0)^A_B. \tag{3.11}$$

Due to the arbitrariness of $\mathbf{G}_0$ it folows from (3.11) that

$$g_{ab}(\mathbf{P})^{bA}(\mathbf{F})^a_B + (\mathbf{J})^{\cdot A}_{\alpha} + (\mathbf{P}^d)^{DA}_{\alpha}\left[(\mathbf{F}^p)^{\alpha}_{D,B} - (\mathbf{F}^p)^{\alpha}_{B,D}\right] = W\delta^A_B. \tag{3.12}$$

It is easy to see that (3.12) is equivalent to (2.25). Thus, the invariance of $\hat{\mathfrak{w}}$ with respect to (1.23) leads to the balance of micromomentum (2.8), which can be written in integral form as follows

$$-\int_{\mathcal{U}_0}\mathbf{J}\,dv + \int_{\partial\mathcal{U}_0}\mathbf{P}^d_{\nu}\,da = \mathbf{0}. \tag{3.13}$$

Let us choose now a family of inhomogeneous initial deformations such that

$$(\mathbf{F}_0^{-1})^A_B = (\mathbf{A}_0)^A_{BC}X^C + (\mathbf{B}_0)^A_B, \quad \mathbf{A}_0, \mathbf{B}_0 = \text{const}, \tag{3.14}$$
$$(\mathbf{A}_0)^A_{BC} = (\mathbf{A}_0)^A_{CB}.$$

Differentiating (3.8) again with respect to α at $\alpha = 0$, then taking the rule (1.27) and the balance of micromomentum (3.12) into account we have

$$(\mathbf{P}^d)^{BC}_{\alpha}(\mathbf{F}^p)^{\alpha}_D(\mathbf{H}_0)^D_{BC} = 0, \tag{3.15}$$

where

$$\mathbf{H}_0 = \frac{d}{d\alpha}\mathbf{A}_0\Big|_{\alpha=0}. \tag{3.16}$$

Since $\mathbf{F}^p$ and $\mathbf{H}_0$ are arbitrary, from (3.16) and $(3.14)_3$ it follows that

$$(\mathbf{P}^d)^{BC}_{\alpha} = -(\mathbf{P}^d)^{CB}_{\alpha}. \tag{3.17}$$

The equation (3.17) is called the balance of moment of micromomentum. In integral form it reads

$$\int_{\mathcal{U}_0}[(\mathbf{P}^d)^{BC}_{\alpha} - (\mathbf{P}^d)^{CB}_{\alpha}]\,dv = 0. \tag{3.18}$$

The balance equations (3.13) and (3.18) can also be derived directly from the principle of virtual work (2.3).

3.4 Equilibrium equations relative to the current and crystal references

Let us write down the balance equations (3.5) and (3.6) relative to the current reference, using the well-known Euler and Piola identities

$$\int_{\partial\phi(\mathcal{U})} \boldsymbol{\sigma}_\nu \, da = \mathbf{0}, \tag{4.1}$$

$$\int_{\partial\phi(\mathcal{U})} \mathbf{x} \times \boldsymbol{\sigma}_\nu \, da = \mathbf{0}, \tag{4.2}$$

where $\boldsymbol{\sigma}_\nu = \boldsymbol{\sigma}\mathbf{n}$, $\boldsymbol{\sigma}$ being the Cauchy stress tensor related to $\mathbf{P}$ by

$$\boldsymbol{\sigma} = J^{-1}\mathbf{P}\mathbf{F}^T, \tag{4.3}$$

In localized form the equations (4.1) and (4.2) read

$$\mathrm{div}\boldsymbol{\sigma} = \mathbf{0}, \tag{4.4}$$

$$\boldsymbol{\sigma}^T = \boldsymbol{\sigma}. \tag{4.5}$$

Let us consider the remaining balance equations for the micromomentum and moment of micromomentum. We introduce the tensors $\mathbf{p}^d$ and $\mathbf{j}$, which are related to $\mathbf{P}^d$ and $\mathbf{J}$ as follows

$$(\mathbf{p}^d)^{bc}_\alpha = J^{-1}(\mathbf{P}^d)^{BC}_\alpha (\mathbf{F})^b_B (\mathbf{F})^c_C, \tag{4.6}$$

$$\mathbf{j} = J^{-1}\mathbf{J}\mathbf{F}^T. \tag{4.7}$$

Expressing $\mathbf{P}^d$ through $\mathbf{p}^d$, then substituting it into (2.8) and using the Piola identity, we get the equation

$$\mathrm{div}\mathbf{p}^d - \mathbf{j} = \mathbf{0}. \tag{4.8}$$

In a similar manner, from (4.6) and (3.17) we get

$$(\mathbf{p}^d)^{bc}_\alpha = -(\mathbf{p}^d)^{cb}_\alpha. \tag{4.9}$$

From the definitions (1.17), (4.3) and (4.6) the expression for the microforce $\mathbf{j}$ follows

$$(\mathbf{j})^{\cdot b}_\alpha = (\mathbf{F}^e)^c_\alpha \left[-(\mathbf{g})_{cd}(\boldsymbol{\sigma})^{db} + \hat{w}\delta^b_c + (\mathbf{t}^e)^a_{cd}(\boldsymbol{\sigma}^d)^{bd}_a\right], \tag{4.10}$$

where $\boldsymbol{\sigma}^d$ is the couple stress tensor, which is related to $\mathbf{p}^d$ by

$$\boldsymbol{\sigma}^p = -\mathbf{F}^{e-T}\mathbf{p}^d, \quad \boldsymbol{\sigma}^d = 2\frac{\partial\hat{w}}{\partial\mathbf{t}^e}. \tag{4.11}$$

It is also possible to express the balance equations relative to the crystal reference. First of all, we shall prove the following identity

$$\operatorname{div}(J^{e-1}\mathbf{F}^{eT}) = J^{e-1}\bar{\boldsymbol{\tau}}, \tag{4.12}$$

with the vector $\bar{\boldsymbol{\tau}}$ given by

$$(\bar{\boldsymbol{\tau}})_\beta = (\bar{\mathbf{t}}^e)^\alpha_{\beta\alpha} = (\mathbf{F}^{e-1})^\alpha_a[(\mathbf{F}^e)^a_{\beta,\alpha} - (\mathbf{F}^e)^a_{\alpha,\beta}]. \tag{4.13}$$

The formula (4.12) generalizes the well-known Piola identity to the anholonomic case (if $\mathbf{F}^e$ were compatible, the right-hand side of (4.12) would vanish, so that it would become the Piola identity). We show (4.12) directly in components, using the definitions of determinant and relative derivative

$$\begin{aligned}(J^{e-1}(\mathbf{F}^e)^b_\beta)_{,b} &= J^{e-1}(\mathbf{F}^e)^a_\alpha(\mathbf{F}^{e-1})^\alpha_{a,b}(\mathbf{F}^e)^b_\beta + J^{e-1}(\mathbf{F}^e)^b_{\beta,b} \\ &= J^{e-1}\left[(\mathbf{F}^e)^a_\alpha(\mathbf{F}^{e-1})^\alpha_{a,\beta} + (\mathbf{F}^e)^a_{\beta,\alpha}(\mathbf{F}^{e-1})^\alpha_a\right] \\ = J^{e-1}\left[-(\mathbf{F}^{e-1})^\alpha_a(\mathbf{F}^e)^a_{\alpha,\beta} + (\mathbf{F}^{e-1})^\alpha_a(\mathbf{F}^e)^a_{\beta,\alpha}\right] &= J^{e-1}(\bar{\boldsymbol{\tau}})_\beta.\end{aligned}$$

We define the stress tensor $\bar{\mathbf{p}}$ as follows

$$\bar{\mathbf{p}} = J^e\boldsymbol{\sigma}\mathbf{F}^{e-T}, \tag{4.14}$$

$$(\bar{\mathbf{p}})^{a\alpha} = J^e(\boldsymbol{\sigma})^{ab}(\mathbf{F}^{e-1})^\beta_b.$$

This tensor plays the same role with respect to the crystal reference as the first Piola-Kirchhoff stress tensor does with respect to the initial configuration. Using (4.14) to express $\boldsymbol{\sigma}$ through $\bar{\mathbf{p}}$ and substituting the result into the balance of macromomentum (4.4) we have

$$(\bar{\mathbf{p}})^{a\beta}_{,\beta} + (\bar{\mathbf{p}})^{a\beta}(\bar{\boldsymbol{\tau}})_\beta = 0, \tag{4.15}$$

or in absolute notation

$$\operatorname{div}_{\bar{\mathbf{K}}_t}\bar{\mathbf{p}} + \bar{\mathbf{p}}\bar{\boldsymbol{\tau}} = \mathbf{0}. \tag{4.16}$$

In deriving (4.15) we have used only the identity (4.12). The equation (4.15) was first obtained by Noll (1967) and Wang (1967). The balance of moment of momentum now becomes

$$\bar{\mathbf{s}}^T = \bar{\mathbf{s}}, \quad \bar{\mathbf{s}} = \mathbf{F}^{e-1}\bar{\mathbf{p}}. \tag{4.17}$$

Let us now introduce the following couple stress tensor relative to the crystal reference

$$(\bar{\mathbf{s}}^d)^{\beta\gamma}_\alpha = -J^e(\mathbf{p}^d)^{be}_\alpha(\mathbf{F}^{e-1})^\beta_b(\mathbf{F}^{e-1})^\gamma_e. \tag{4.18}$$

Substituting $\mathbf{p}^d$ expressed as function of $\bar{\mathbf{s}}^d$ into the balance equation (4.8) and using the identity (4.12), one can see that

$$(\mathbf{p}^d)^{bc}_{\alpha,e} - (\mathbf{j})^b_\alpha = -J^{e-1}\left[(\bar{\mathbf{s}}^d)^{\beta\gamma}_{\alpha,\gamma}(\mathbf{F}^e)^b_\beta + (\bar{\mathbf{s}}^d)^{\beta\gamma}_\alpha(\mathbf{F}^e)^b_{\beta,\gamma}\right.$$
$$\left.+(\bar{\mathbf{s}}^d)^{\beta\gamma}_\alpha(\mathbf{F}^e)^b_\beta(\bar{\tau})_\gamma\right] - (\mathbf{j})^b_\alpha = 0. \tag{4.19}$$

Multiplying this equation by $J^e(\mathbf{F}^{e-1})^\delta_b$ and using the definition of the torsion tensor (1.4.15) we obtain

$$(\bar{\mathbf{s}}^d)^{\delta\gamma}_{\alpha,\gamma} + (\bar{\mathbf{s}}^d)^{\beta\gamma}_\alpha(\bar{\mathbf{t}})^\delta_{\beta\gamma} + (\bar{\mathbf{s}}^d)^{\delta\gamma}_\alpha(\bar{\tau})_\gamma - (\bar{\mathbf{j}})^\delta_\alpha = 0, \tag{4.20}$$

where

$$(\bar{\mathbf{j}})^\delta_\alpha = J^e(\mathbf{j})^b_\alpha(\mathbf{F}^{e-1})^\delta_b. \tag{4.21}$$

Using (1.17), (4.14), (4.17) and (4.18) it is easy to show that

$$(\bar{\mathbf{j}})^\delta_\alpha = -(\bar{\mathbf{c}}^e)_{\alpha\beta}(\bar{\mathbf{s}})^{\beta\delta} + \bar{\mathfrak{w}}\delta^\delta_\alpha + (\bar{\mathbf{t}})^\gamma_{\alpha\beta}(\bar{\mathbf{s}}^d)^{\delta\beta}_\gamma. \tag{4.22}$$

The balance of moment of micromomentum results now from (4.9) and (4.18) to be

$$(\bar{\mathbf{s}}^d)^{\beta\gamma}_\alpha = (\bar{\mathbf{s}}^d)^{\gamma\beta}_\alpha. \tag{4.23}$$

Chapter 4

Dynamics

4.1 Principle of stationary action

One can generalize to dynamics the results obtained in Chapter 3 in a straightforward manner by introducing the kinetic energy and formulating the variational principle of stationary action. We assume the existence of an action functional of an elastoplastic body with microstructure which is given in the form

$$I[\mathbf{x}, \mathbf{F}^p] = \int_0^T \int_{\mathcal{B}_0} \mathcal{L}(\dot{\mathbf{x}}, \dot{\mathbf{F}}^p; \mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p)\, dv\, dt, \tag{1.1}$$

where

$$\mathcal{L}(\dot{\mathbf{x}}, \dot{\mathbf{F}}^p; \mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p) = \rho_0[K(\dot{\mathbf{x}}, \dot{\mathbf{F}}^p) - E(\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p)]. \tag{1.2}$$

The function $\mathcal{L}$, called the Lagrangian, is the difference of the kinetic energy density $\rho_0 K$ and the internal energy density $\rho_0 E(\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p)$ per unit initial volume, where $\rho_0(\mathbf{X}) = \mathfrak{r}_0(X)$ is the mass density. The kinetic energy density per unit mass can be specified by

$$K(\dot{\mathbf{x}}, \dot{\mathbf{F}}^p) = \frac{1}{2} g_{ab} \dot{x}^a \dot{x}^b + \frac{1}{2} g_{\alpha\beta} \Xi^{AB} (\dot{\mathbf{F}}^p)^\alpha_A (\dot{\mathbf{F}}^p)^\beta_B, \tag{1.3}$$

where Ξ^{AB} is a constant symmetric tensor of second rank. The first term of (1.3) corresponds to the kinetic energy of the macromotion, while its second term corresponds to the kinetic energy of the dislocation motion. As about the internal energy density per unit initial volume, we shall assume, as we did in Chapter 3, that it depends on $\mathbf{F}^p$, $\mathbf{C}$ and $\mathbf{T}^p$ in such a way that

$$\rho_0 E = \rho_0 \hat{E}(\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p) = J^p \hat{\mathbf{e}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \bar{\mathbf{t}}(\mathbf{F}^p, \mathbf{T}^p)), \tag{1.4}$$

where $\hat{\mathbf{e}}(\bar{\mathbf{c}}^e, \bar{\mathbf{t}})$ is the internal energy per unit crystal volume which is the function of $\bar{\mathbf{c}}^e$ and $\bar{\mathbf{t}}$ *alone* (cf. formula (3.1.20) for the free energy density).

This means that the internal energy density is invariant with respect to the superposed rigid-body motion, and also with respect to the rescaling group (3.1.23) (up to the factor J^p).

Assuming the absence of external body forces and surface tractions we formulate the principle of stationary action as follows

$$\delta I[\mathbf{x}, \mathbf{F}^p] = 0. \tag{1.5}$$

Here the variation of the functional I is defined analogously as in (3.4.2). We calculate now the variation of the action functional (1.1)

$$\delta I = \int_0^T \int_{\mathcal{B}_0} \left[\rho_0 \mathbf{M} \cdot \delta\dot{\mathbf{x}} + \rho_0 < \mathbf{M}^d, \delta\dot{\mathbf{F}}^p > - < \mathbf{gP}, \delta D\mathbf{x} > \right.$$

$$\left. - < \mathbf{J}, \delta\mathbf{F}^p > - < \mathbf{P}^d, \delta D\mathbf{F}^p > \right] dv\, dt. \tag{1.6}$$

In (1.6) the following fields are introduced

$$\mathbf{M} = \mathbf{g}^{-1} \frac{\partial K}{\partial \dot{\mathbf{x}}}\bigg|_{\dot{\mathbf{F}}^p} = \dot{\mathbf{x}}, \tag{1.7}$$

$$\mathbf{M}^d = \frac{\partial K}{\partial \dot{\mathbf{F}}^p}\bigg|_{\dot{\mathbf{x}}},$$

$$(\mathbf{M}^d)^A_\alpha = g_{\alpha\beta} \Xi^{AB} (\dot{\mathbf{F}}^p)^\beta_B, \tag{1.8}$$

$$\mathbf{P} = \rho_0\, \mathbf{g}^{-1} \frac{\partial E}{\partial \mathbf{F}}\bigg|_{\mathbf{F}^p, D\mathbf{F}^p}, \tag{1.9}$$

$$\mathbf{J} = \rho_0 \frac{\partial E}{\partial \mathbf{F}^p}\bigg|_{\mathbf{F}, D\mathbf{F}^p}, \tag{1.10}$$

$$\mathbf{P}^d = \rho_0 \frac{\partial E}{\partial D\mathbf{F}^p}\bigg|_{\mathbf{F}, \mathbf{F}^p}. \tag{1.11}$$

We call $\mathbf{M}$ the momentum of macromotion (the macromomentum), $\mathbf{M}^d$ the momentum of dislocation motion (the micromomentum, for short), $\mathbf{P}$ the macrostress tensor, $\mathbf{J}$ the internal microforce tensor, and $\mathbf{P}^d$ the microstress tensor.

Integrating (1.6) by parts and assuming that the variations on the boundary $\partial\mathcal{U}_0$ and at $t = 0, T$ vanish we obtain

$$\delta I = \int_0^T \int_{\mathcal{B}_0} \left[(-\rho_0 \dot{\mathbf{M}} + \mathrm{Div}\mathbf{P}) \cdot \delta\mathbf{x} \right.$$

$$+ < (-\rho_0 \dot{\mathbf{M}}^d + \mathrm{Div}\mathbf{P}^d - \mathbf{J}), \delta\mathbf{F}^p > \Big]\, dv\, dt = 0. \tag{1.12}$$

Since $\delta\mathbf{x}$ and $\delta\mathbf{F}^p$ are arbitrary, from (1.12) we get the following equations of motion

$$\rho_0 \dot{\mathbf{M}} = \mathrm{Div}\mathbf{P} \quad \text{(macromotion)}, \tag{1.13}$$

$$\rho_0 \dot{\mathbf{M}}^d = \mathrm{Div}\mathbf{P}^d - \mathbf{J} \quad \text{(dislocation motion)}. \tag{1.14}$$

From (1.4) and the definitions (1.9)-(1.11) one can derive the following constitutive relations

$$\mathbf{P} = \mathbf{F}\mathbf{S}, \qquad \mathbf{S} = 2\rho_0 \frac{\partial \hat{E}}{\partial \mathbf{C}} = J^p \mathbf{F}^{p-1} \bar{\mathbf{s}} \mathbf{F}^{p-T}, \tag{1.15}$$

$$\bar{\mathbf{s}} = 2\frac{\partial \hat{\bar{\mathbf{e}}}}{\partial \bar{\mathbf{c}}^e}, \tag{1.16}$$

$$\mathbf{P}^d = -\mathbf{F}^{p-T}\mathbf{S}^d, \qquad \mathbf{S}^d = 2\rho_0 \frac{\partial \hat{E}}{\partial \mathbf{T}^p}, \tag{1.17}$$

$$\mathbf{S}^d(\mathbf{W}) = J^p \mathbf{F}^{p-1} \bar{\mathbf{s}}^d(\bar{\mathbf{w}}) \mathbf{F}^{p-T}, \tag{1.18}$$

$$\bar{\mathbf{s}}^d = 2\frac{\partial \hat{\bar{\mathbf{e}}}}{\partial \bar{\mathbf{t}}}, \tag{1.19}$$

$$(\mathbf{J})^{.A}_{\alpha} = (\mathbf{F}^{p-1})^C_{\alpha} \Big[-(\mathbf{C})_{CD} (\mathbf{S})^{DA} + \rho_0 \hat{E} \delta^A_C + (\mathbf{T}^p)^B_{CD} (\mathbf{S}^d)^{DA}_B \Big]. \tag{1.20}$$

The equations (1.13)-(1.19) constitute the complete system of relations with respect to the unknown functions $\mathbf{x}$ and $\mathbf{F}^p$. In order to make the problem well-posed we must additionally specify the boundary and initial conditions in a similar way as in classical elasticity.

As about the internal energy density, the action functional (1.1) is invariant with respect to the groups of translation and rotation of the Euclidean space $\mathcal{E}$. Therefore, applying Noether's theorem (see, e.g., Marsden & Hughes 1983) we can derive again (1.13) and the following equation

$$\mathbf{P}\mathbf{F}^T = \mathbf{F}\mathbf{P}^T, \tag{1.21}$$

which represent the balance laws of macromomentum and moment of macromomentum for the stationary points. Besides, the internal energy density $\bar{\mathbf{e}}(\bar{\mathbf{c}}^e, \bar{\mathbf{t}})$ is invariant with respect to the rescaling group (3.1.23). Therefore, repeating the same procedure as in Section 3.3, one can derive the equations (3.3.12) and (3.3.17). The equation (3.3.12) can be referred to as either the balance of micromomentum, or the definition of the microforce.

The equation (3.3.17) corresponds to the balance of moment of micromomentum.

All these balance laws can be formulated in integral form as follows

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\mathbf{M}\,dv=\int_{\partial\mathcal{U}_0}\mathbf{P}_\nu\,da\quad\text{(macromomentum)},\tag{1.22}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\mathbf{x}\times\mathbf{M}\,dv=\int_{\partial\mathcal{U}_0}\mathbf{x}\times\mathbf{P}_\nu\,da$$

$$\text{(moment of macromomentum)},\tag{1.23}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\mathbf{M}^d\,dv=-\int_{\mathcal{U}_0}\mathbf{J}\,dv+\int_{\partial\mathcal{U}_0}\mathbf{P}^d_\nu\,da\quad\text{(micromomentum)},\tag{1.24}$$

$$\int_{\mathcal{U}_0}[(\mathbf{P}^d)^{BC}_\alpha+\mathbf{P}^d)^{CB}_\alpha]\,dv=0,\quad\text{(moment of micromomentum)},\tag{1.25}$$

for an arbitrary sub-body $\mathcal{U}$, with the microforce $\dot{\mathbf{J}}$ given by (1.20). Finally, using the equations of motion (1.13) and (1.14) one can establish the balance of energy

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0(K+E)\,dv=\int_{\partial\mathcal{U}_0}[\mathbf{P}_\nu\cdot\dot{\mathbf{x}}+<\mathbf{P}^d_\nu,\dot{\mathbf{F}}^p>]\,da\quad\text{(energy)}.\tag{1.26}$$

The right-hand side of (1.26) corresponds to the power done by the external forces. One can see that the internal microforce does not contribute to this power. To prove (1.26) let us expand its left-hand side

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0(K+E)\,dv=\int_{\mathcal{U}_0}(\rho_0\dot{\mathbf{M}}\cdot\dot{\mathbf{x}}+<\rho_0\dot{\mathbf{M}}^d,\dot{\mathbf{F}}^p>)\,dv$$

$$+\int_{\mathcal{U}_0}(<\mathbf{gP},\dot{\mathbf{F}}>+<\mathbf{J},\dot{\mathbf{F}}^p>+<\mathbf{P}^d,D\dot{\mathbf{F}}^p>)\,dv,\tag{1.27}$$

then use the equations of motions (1.13) and (1.14) to replace the first integral in (1.27) by

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0K\,dv=\int_{\mathcal{U}_0}(\mathrm{Div}\mathbf{P}\cdot\dot{\mathbf{x}}+<-\mathbf{J}+\mathrm{Div}\mathbf{P}^d,\dot{\mathbf{F}}^p>)\,dv.\tag{1.28}$$

Substituting now (1.28) into (1.27), canceling equal terms and integrating by parts one gets the right-hand side of (1.26).

4.2 Balance equations in the initial description

In the previous Section we dealt only with the purely mechanical theory. In general, the plastic deformation may be accompanied by the heat flux and the change of temperature. In such cases the principle of stationary action formulated above is no more adequate. We shall generalize now the balance equations so that the heat flux and the Clausius-Duhem inequality can be included in a natural manner.

Let $\rho_0(\mathbf{X}) = \mathfrak{r}_0(X,0)$ be the mass density, $\dot{\mathbf{x}}(\mathbf{X},t)$ the velocity, $\mathbf{M}(\mathbf{X},t)$ the macromomentum,$\mathbf{M}^d(\mathbf{X},t)$ the micromomentum, $\mathbf{P}(\mathbf{X},t)$ the first Piola-Kirchhoff stress tensor, $\mathbf{J}(\mathbf{X},t)$ the driving force , $\mathbf{P}^d(\mathbf{X},t)$ the microstress, $K(\mathbf{X},t)$ the kinetic energy density and $E(\mathbf{X},t)$ the internal energy density, both per unit mass, $\mathbf{Q}(\mathbf{X},t)$ the heat flux vector, $\Theta(\mathbf{X},t)$ the temperature, and $N(\mathbf{X},t)$ the entropy density per unit initial volume. Now we postulate the following balance equations

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\,dv = 0 \quad \text{(mass)}, \tag{2.1}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\mathbf{M}\,dv = \int_{\partial\mathcal{U}_0}\mathbf{P}_\nu\,da \quad \text{(macromomentum)}, \tag{2.2}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\mathbf{x}\times\mathbf{M}\,dv = \int_{\partial\mathcal{U}_0}\mathbf{x}\times\mathbf{P}_\nu\,da$$
$$\text{(moment of macromomentum)}, \tag{2.3}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0\mathbf{M}^d\,dv = -\int_{\mathcal{U}_0}\mathbf{J}\,dv + \int_{\partial\mathcal{U}_0}\mathbf{P}^d_\nu\,da \quad \text{(micromomentum)}, \tag{2.4}$$

$$\int_{\mathcal{U}_0}[(\mathbf{P}^d)^{BC}_\alpha + \mathbf{P}^d)^{CB}_\alpha]\,dv = 0 \quad \text{(moment of micromomentum)}, \tag{2.5}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0(K+E)\,dv = \int_{\partial\mathcal{U}_0}[\mathbf{P}_\nu\cdot\dot{\mathbf{x}} + < \mathbf{P}^d_\nu, \dot{\mathbf{F}}^p > -\mathbf{Q}_\nu]\,da$$
$$\text{(energy)}, \tag{2.6}$$

$$\frac{d}{dt}\int_{\mathcal{U}_0}\rho_0 N\,dv \geq -\int_{\partial\mathcal{U}_0}\frac{\mathbf{Q}_\nu}{\Theta}\,da \quad \text{(entropy)}, \tag{2.7}$$

for an arbitrary sub-body $\mathcal{U}$. In comparison with (1.26) the balance of energy is generalized to account for the heat flux. The inequality (2.7) is new and corresponds to the entropy production inequality in integral form. Standard procedures enable one to pass to the localized form of the

balance equations. The localized equations of (2.1)-(2.5) can be written immediately

$$\rho_0 = \text{const} \quad \text{(mass)}, \tag{2.8}$$

$$\rho_0 \dot{\mathbf{M}} = \text{Div}\mathbf{P} \quad \text{(macromomentum)}, \tag{2.9}$$

$$\mathbf{S} = \mathbf{S}^T, \quad \mathbf{P} = \mathbf{F}\mathbf{S} \quad \text{(moment of macromomentum)}, \tag{2.10}$$

$$\rho_0 \dot{\mathbf{M}}^d = \text{Div}\mathbf{P}^d - \mathbf{J} \quad \text{(micromomentum)}, \tag{2.11}$$

$$(\mathbf{P}^d)_\alpha^{BC} = -(\mathbf{P}^d)_\alpha^{CB} \quad \text{(moment of micromomentum)}. \tag{2.12}$$

We show now how the balance of energy and the entropy inequality in localized form can be obtained. Integrating (2.6) by parts we obtain

$$\frac{d}{dt}\int_{\mathcal{U}_0} \rho_0(K+E)\,dv = \int_{\mathcal{U}_0}[\text{Div}\mathbf{P}\cdot\dot{\mathbf{x}} + <\mathbf{g}\mathbf{P}, \dot{\mathbf{F}}> + <\text{Div}\mathbf{P}^d, \dot{\mathbf{F}}^p> + <\mathbf{P}^d, D\dot{\mathbf{F}}^p> - \text{Div}\mathbf{Q}]\,da. \tag{2.13}$$

Using the equation (1.28) to subtract the rate of the kinetic energy from (2.13), we have

$$\frac{d}{dt}\int_{\mathcal{U}_0} \rho_0 E\,dv = \int_{\mathcal{U}_0}[<\mathbf{g}\mathbf{P}, \dot{\mathbf{F}}> + <\mathbf{J}, \dot{\mathbf{F}}^p> + <\mathbf{P}^d, D\dot{\mathbf{F}}^p> - \text{Div}\mathbf{Q}]\,da. \tag{2.14}$$

Since (2.14) should hold for an arbitrary subbody $\mathcal{U}_0$, the localized form of the balance of energy follows

$$\rho_0\dot{E} + \text{Div}\mathbf{Q} = <\mathbf{g}\mathbf{P}, \dot{\mathbf{F}}> + <\mathbf{J}, \dot{\mathbf{F}}^p> + <\mathbf{P}^d, D\dot{\mathbf{F}}^p> \quad \text{(energy)}. \tag{2.15}$$

In (2.15) we regard the internal energy per unit mass as the function of $\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p$ and the entropy N. This balance equation can also be written in a slightly different form. We note that

$$\mathbf{D} = \frac{1}{2}\dot{\mathbf{C}} = \frac{1}{2}(\dot{\mathbf{F}}^T\mathbf{g}\mathbf{F} + \mathbf{F}^T\mathbf{g}\dot{\mathbf{F}}), \tag{2.16}$$

$$\mathbf{Z}(\mathbf{W}_1, \mathbf{W}_2) = \frac{1}{2}\dot{\mathbf{T}}^p(\mathbf{W}_1, \mathbf{W}_2) = -\frac{1}{2}\mathbf{F}^{p-1}\dot{\mathbf{F}}^p[\mathbf{T}^p(\mathbf{W}_1, \mathbf{W}_2)] + \frac{1}{2}\mathbf{F}^{p-1}[((D\dot{\mathbf{F}}^p)\mathbf{W}_2)\mathbf{W}_1 - ((D\dot{\mathbf{F}}^p)\mathbf{W}_1)\mathbf{W}_2]. \tag{2.17}$$

We replace now $\mathbf{P}$ and $\mathbf{P}^d$ in the right-hand side of (2.15) by $\mathbf{S}$ and $\mathbf{S}^d$ according to $(1.15)_1$ and $(1.17)_1$. Using (2.16) and (2.17) we transform the balance of energy to

$$\rho_0\dot{E} + \text{Div}\mathbf{Q} = < \mathbf{S}, \mathbf{D} > + < \tilde{\mathbf{J}}, \dot{\mathbf{F}}^p > + < \mathbf{S}^d, \mathbf{Z} > \quad \text{(energy)}, \tag{2.18}$$

where

$$\tilde{\mathbf{J}} = \mathbf{J} + \frac{1}{2}\mathbf{F}^{p-T}(\mathbf{S}^d\colon \mathbf{T}^p),$$

$$(\tilde{\mathbf{J}})^A_\alpha = (\mathbf{J})^A_\alpha + \frac{1}{2}(\mathbf{F}^{p-1})^C_\alpha[(\mathbf{S}^d)^{BD}_C(\mathbf{T}^p)^A_{BD}]. \tag{2.19}$$

The interpretation of $\tilde{\mathbf{J}}$ can be given in the context of the balance of energy (2.18), where the internal energy per unit mass is regarded as the function of $\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p$ and N

$$E = \hat{E}(\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p, N) = J^p\hat{\mathfrak{e}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \bar{\mathbf{t}}(\mathbf{F}^p, \mathbf{T}^p), \bar{\eta}). \tag{2.20}$$

We shall show in the next Chapter that

$$\tilde{\mathbf{J}} = \rho_0 \frac{\partial \hat{E}}{\partial \mathbf{F}^p}\bigg|_{\mathbf{C},\mathbf{T}^p,N}.$$

In a similar way, from (2.7) we obtain the localized entropy production inequality

$$\rho_0\dot{N} \geq -\frac{\text{Div}\mathbf{Q}}{\Theta} + < \frac{\text{Grad}\Theta}{\Theta^2}, \mathbf{Q} > . \tag{2.21}$$

We introduce the free energy per unit mass as follows

$$\Psi = E - N\Theta. \tag{2.22}$$

This is regarded as a function of $\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p$ and the temperature Θ. The time derivative of (2.22) gives

$$\dot{\Psi} = \dot{E} - \dot{N}\Theta - N\dot{\Theta},$$

or

$$\Theta\dot{N} = \dot{E} - N\dot{\Theta} - \dot{\Psi}. \tag{2.23}$$

Combining (2.23) with (2.21) and noting that Θ is positive we have

$$\rho_0(\dot{E} - N\dot{\Theta} - \dot{\Psi}) \geq -\text{Div}\mathbf{Q} + < \frac{\text{Grad}\Theta}{\Theta}, \mathbf{Q} > . \tag{2.24}$$

Substitution of $\dot{E}$ from (2.15) into (2.24) gives

$$\rho_0(N\dot{\Theta}+\dot{\Psi})- < \mathbf{gP},\dot{\mathbf{F}} > - < \mathbf{J},\dot{\mathbf{F}}^p >$$

$$- < \mathbf{P}^d, D\dot{\mathbf{F}}^p > + < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} > \leq 0. \tag{2.25}$$

The inequality (2.25) is referred to as the localized form of the entropy production inequality, which can and should restrict the possible functional form of the constitutive equations. Using (2.18) we can rewrite (2.25) in a sightly different form

$$\rho_0(N\dot{\Theta}+\dot{\Psi})- < \mathbf{S},\mathbf{D} > - < \tilde{\mathbf{J}},\dot{\mathbf{F}}^p >$$

$$- < \mathbf{S}^d, \mathbf{Z} > + < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} > \leq 0, \tag{2.26}$$

with $\tilde{\mathbf{J}}$ given by (2.19). The free energy per unit mass in (2.26) is regarded as a function of $\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p$ and Θ

$$\Psi = \hat{\Psi}(\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p, \Theta) = J^p \hat{\mathfrak{w}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \bar{\mathbf{t}}(\mathbf{F}^p, \mathbf{T}^p), \bar{\theta}). \tag{2.27}$$

4.3 Balance equations in the current description

For numerical implementations, the formulation of the balance laws and of the entropy production inequality relative to the current reference is of major importance. Let $\rho(\mathbf{x},t) = \mathfrak{r}(X,t)$ be the mass density, $\mathbf{v}(\mathbf{x},t)$ the spatial velocity field and $\boldsymbol{\sigma}(\mathbf{x},t)$ the Cauchy stress tensor. Standard procedures with the use of the Euler and Piola identities enable one to transform (2.8)-(2.10) to the following balance equations

$$D_t\rho + \rho\ \mathrm{div}\mathbf{v} = 0 \quad \text{(mass)}, \tag{3.1}$$

$$\rho D_t\mathbf{v} = \rho\mathbf{b} + \ \mathrm{div}\boldsymbol{\sigma} \quad \text{(macromomentum)}, \tag{3.2}$$

$$\boldsymbol{\sigma}^T = \boldsymbol{\sigma} \quad \text{(moment of macromomentum)}. \tag{3.3}$$

with D_t the material time derivative. The Cauchy stress tensor is related to the first Piola-Kichhoff stress tensor by (3.4.3).

We consider now the balance of micromomentum and moment of micromomentum. Introducing the microstress tensor $\mathbf{p}^d$ and the driving force

tensor $\mathbf{j}$ as in (3.4.6) and (3.4.7) and using the Piola identity, we reduce (2.11) to

$$\rho_0 \dot{\mathbf{M}}^d = J(\mathrm{div}\mathbf{p}^d)\mathbf{F}^{-T} - J\mathbf{j}\mathbf{F}^{-T} \tag{3.4}$$

Multiplying (3.4) by $J^{-1}\mathbf{F}^T$ gives

$$\rho\boldsymbol{\mu} = \mathrm{div}\mathbf{p}^d - \mathbf{j} \quad \text{(micromomentum)}, \tag{3.5}$$

where

$$\boldsymbol{\mu} = \dot{\mathbf{M}}\mathbf{F}^T. \tag{3.6}$$

It is easy to see that the balance of moment of micromomentum becomes

$$(\mathbf{p}^d)^{bc}_{\alpha} = -(\mathbf{p}^d)^{cb}_{\alpha} \quad \text{(moment of micromomentum)}. \tag{3.7}$$

Let us consider now the balance of energy. We use e to denote the internal energy per unit mass, which is regarded as a function of $\mathbf{F}^{e-1}, \mathbf{g}, \mathbf{t}^e$ and the entropy η

$$e = \hat{e}(\mathbf{F}^{e-1}, \mathbf{g}, \mathbf{t}^e, \eta). \tag{3.8}$$

Since e is a scalar, it should not change its values under the change of reference. Therefore the material time derivative of e should equal $\dot{E}$

$$D_t e = \dot{E}. \tag{3.9}$$

We introduce the tensors $\boldsymbol{\sigma}, \boldsymbol{\sigma}^d, \tilde{\mathbf{j}}$ and $\mathbf{q}$ given by (3.4.3), (3.4.11) and

$$(\tilde{\mathbf{j}})^a_{\alpha} = (\mathbf{j})^a_{\alpha} + \frac{1}{2}(\mathbf{F}^e)^c_{\alpha}[(\boldsymbol{\sigma}^d)^{bd}_{e}(\mathbf{t}^e)^a_{bd}], \tag{3.10}$$

$$\mathbf{q} = J^{-1}\mathbf{F}\mathbf{Q}. \tag{3.11}$$

Multiplying the balance of energy (2.18) by J^{-1} and taking into account (3.9)-(3.11) we can transform (2.18) to

$$\begin{aligned} \rho D_t e + \ \mathrm{div}\mathbf{q} \ =& < \boldsymbol{\sigma}, \mathbf{d} > + < \tilde{\mathbf{j}}, \bar{\mathbf{l}}^p \mathbf{F}^{e-1} > \\ &+ < \boldsymbol{\sigma}^d, \mathbf{z} > \quad \text{(energy)}, \end{aligned} \tag{3.12}$$

with $\mathbf{d}$ denoting the total strain rate tensor and $\mathbf{z}$ the dislocation drift rate tensor.

We introduce the free energy per unit mass as follows

$$\psi = e - \eta\theta, \tag{3.13}$$

with θ denoting the temperature field. We can rewrite the entropy production inequality (2.26) in the following form

$$\rho(\eta D_t\theta + D_t\psi) - < \boldsymbol{\sigma}, \mathbf{d} > - < \tilde{\mathbf{j}}, \bar{\mathbf{l}}^p \mathbf{F}^{e-1} >$$

$$- < \boldsymbol{\sigma}^d, \mathbf{z} > + < \frac{\text{grad}\theta}{\theta}, \mathbf{q} > \leq 0. \tag{3.14}$$

In the next Chapter we shall derive the constitutive equations consistent with (3.14).

Chapter 5

Constitutive equations: general theory and special cases

5.1 Thermodynamic considerations

In this Section we investigate the consequences of the entropy production inequality written relative to the initial reference according to (3.2.25)

$$\rho_0(N\dot{\Theta}+\dot{\Psi})- < \mathbf{gP}, \dot{\mathbf{F}} > - < \mathbf{J}, \dot{\mathbf{F}}^p >$$

$$- < \mathbf{P}^d, D\dot{\mathbf{F}}^p > + < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} > \leq 0, \tag{1.1}$$

where $\mathbf{P}, \mathbf{P}^d$, and $\mathbf{J}$ are the first Piola-Kirchhoff stress tensor, the microstress tensor, and the driving force tensor, respectively. We assume that the entropy production inequality (1.1) holds for any regular motion of the body with dislocations. Furthermore, according to (4.1.4) and (4.2.22) the free energy Ψ per unit mass should have the following functional form

$$\Psi = \Psi(\mathbf{F}, \mathbf{F}^p, D\mathbf{F}^p, \Theta). \tag{1.2}$$

Let us calculate the rate of the free energy

$$\dot{\Psi} = < \frac{\partial \Psi}{\partial \mathbf{F}}, \dot{\mathbf{F}} > + < \frac{\partial \Psi}{\partial \mathbf{F}^p}, \dot{\mathbf{F}}^p > + < \frac{\partial \Psi}{\partial D\mathbf{F}^p}, D\dot{\mathbf{F}}^p > + \frac{\partial \Psi}{\partial \Theta}\dot{\Theta}, \tag{1.3}$$

where $\partial\Psi/\partial\mathbf{F}$ is the partial derivative of Ψ with respect to $\mathbf{F}$. Substituting the formula (1.3) into the entropy production inequality (1.1) gives

$$< (\rho_0 \frac{\partial \Psi}{\partial \mathbf{F}} - \mathbf{gP}), \dot{\mathbf{F}} > + < (\rho_0 \frac{\partial \Psi}{\partial \mathbf{F}^p} - \mathbf{J}), \dot{\mathbf{F}}^p >$$

$$+ < (\rho_0 \frac{\partial \Psi}{\partial D\mathbf{F}^p} - \mathbf{P}^d), D\dot{\mathbf{F}}^p >$$

$$+\rho_0(\frac{\partial\Psi}{\partial\Theta}+N)\dot{\Theta}+<\frac{\mathrm{Grad}\Theta}{\Theta},\mathbf{Q}>\leq 0. \tag{1.4}$$

Now we apply a procedure due to Coleman and Noll (1963) to derive the following constitutive equations

$$\mathbf{P}=\rho_0\mathbf{g}^{-1}\frac{\partial\Psi}{\partial\mathbf{F}}\Big|_{\mathbf{F}^p,D\mathbf{F}^p,\Theta}, \tag{1.5}$$

$$\mathbf{J}=\rho_0\frac{\partial\Psi}{\partial\mathbf{F}^p}\Big|_{\mathbf{F},D\mathbf{F}^p,\Theta}, \tag{1.6}$$

$$\mathbf{P}^d=\rho_0\frac{\partial\Psi}{\partial D\mathbf{F}^p}\Big|_{\mathbf{F},\mathbf{F}^p,\Theta}, \tag{1.7}$$

$$N=-\frac{\partial\Psi}{\partial\Theta}\Big|_{\mathbf{F},\mathbf{F}^p,D\mathbf{F}^p}. \tag{1.8}$$

By assumption, (1.1) holds for all processes $(\phi_t,\mathbf{F}^p,D\mathbf{F}^p,\Theta)$. First of all, choose ϕ_t and $\mathbf{F}^p$ independent of time; then we must have

$$\rho_0(\frac{\partial\Psi}{\partial\Theta}+N)\dot{\Theta}+<\frac{\mathrm{Grad}\Theta}{\Theta},\mathbf{Q}>\leq 0. \tag{1.9}$$

Suppose $(\partial\Psi/\partial\Theta+N)\dot{\Theta}$ did not vanish for some $\phi,\mathbf{F}^p$ and all $\Theta(\mathbf{X},t)$. Then we can alter Θ to a new one Θ' so that $\Theta(\mathbf{X},t_0)=\Theta'(\mathbf{X},t_0)$ and $\dot{\Theta}(\mathbf{X},t_0)=\alpha\dot{\Theta}'(\mathbf{X},t_0)$, where α is any prescribed constant. We can then choose the constant α to violate the assumed inequality. Therefore, we deduce the relation (1.8). Fixing $\mathbf{F}^p$ and Θ and altering ϕ_t we can derive the equation (1.5). Now fixing Θ and choosing $\mathbf{F}^p$ homogeneous and arbitrary so that $D\mathbf{F}^p=\mathbf{0}$, we get (1.6). The equation (1.7) can be deduced now by fixing Θ and altering $\mathbf{F}^p$ in an arbitrary manner.

By (1.5)-(1.8) we reduce the entropy inequality (1.1) to

$$<\frac{\mathrm{Grad}\Theta}{\Theta},\mathbf{Q}>\leq 0. \tag{1.10}$$

This inequality can be satisfied, for example, by the Fourier law

$$\mathbf{Q}=-\boldsymbol{\kappa}\ \mathrm{Grad}\Theta, \tag{1.11}$$

with $\boldsymbol{\kappa}$ denoting a symmetric tensor of second rank, which is positive definite. After (1.5)-(1.8) the balance of energy reduces to

$$\rho_0\Theta\dot{N}+\mathrm{Div}\mathbf{Q}=\rho_0 R. \tag{1.12}$$

Eqn. (1.12) can be considered as a nonlinear heat conduction equation.

In the finite elastoplasticity with microstructure the free energy has but a more specific form

$$\Psi = \rho_0^{-1} J^p \hat{\mathfrak{w}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \bar{\mathbf{t}}(\mathbf{F}^p, \mathbf{T}^p), \Theta) = \hat{\Psi}(\mathbf{F}^p, \mathbf{C}, \mathbf{T}^p, \Theta), \tag{1.13}$$

with $\hat{\mathfrak{w}}(\bar{\mathbf{c}}^e, \bar{\mathbf{t}})$ the free energy per unit volume of the crystal reference satisfying the principles of frame indifference and initial scaling indifference. Repeating the calculations like those in Section 3.2 one can show that (1.5)-(1.7) are equivalent to

$$\mathbf{S} = 2\rho_0 \frac{\partial \hat{\Psi}}{\partial \mathbf{C}}\bigg|_{\mathbf{F}^p, \mathbf{T}^p, \Theta}, \tag{1.14}$$

$$(\mathbf{J})_\alpha^A = (\mathbf{F}^{p-1})_\alpha^C \left[-(\mathbf{C})_{CD} (\mathbf{S})^{DA} + \rho_0 \hat{\Psi}\, \delta_C^A + (\mathbf{T}^p)_{CD}^B (\mathbf{S}^d)_B^{DA} \right], \tag{1.15}$$

$$\mathbf{S}^d = 2\rho_0 \frac{\partial \hat{\Psi}}{\partial \mathbf{T}^p}\bigg|_{\mathbf{F}^p, \mathbf{C}, \Theta}. \tag{1.16}$$

One can show that the tensor $\tilde{\mathbf{J}}$ given by (4.2.19) can be calculated as follows

$$\tilde{\mathbf{J}} = \rho_0 \frac{\partial \hat{\Psi}}{\partial \mathbf{F}^p}\bigg|_{\mathbf{C}, \mathbf{T}^p, \Theta}. \tag{1.17}$$

We prove (1.17) directly in components. Applying the rule of differentiation for the composite function $\hat{\Psi}$ from (1.13) we have

$$\begin{aligned} (\mathbf{J})_\alpha^A = \rho_0 \frac{\partial \Psi}{\partial (\mathbf{F}^p)_A^\alpha}\bigg|_{\mathbf{F}, D\mathbf{F}^p, \Theta} &= \rho_0 \frac{\partial \hat{\Psi}}{\partial (\mathbf{F}^p)_A^\alpha}\bigg|_{\mathbf{C}, \mathbf{T}^p, \Theta} \\ &+ \rho_0 \frac{\partial \hat{\Psi}}{\partial (\mathbf{T}^p)_{CD}^B}\bigg|_{\mathbf{F}^p, \mathbf{C}, \Theta} \frac{\partial (\mathbf{T}^p)_{CD}^B}{\partial (\mathbf{F}^p)_A^\alpha}\bigg|_{D\mathbf{F}^p}. \end{aligned} \tag{1.18}$$

Using the formulae (1.4.8) and (3.2.20) it is easy to see that

$$\frac{\partial (\mathbf{T}^p)_{CD}^B}{\partial (\mathbf{F}^p)_A^\alpha}\bigg|_{D\mathbf{F}^p} = -(\mathbf{F}^{p-1})_\alpha^B (\mathbf{T}^p)_{CD}^A. \tag{1.19}$$

Substituting (1.19) into (1.18) and recalling (4.2.19) and (1.16) we get (1.17).

By using push-forward operations with $\mathbf{F}$ we can get the following constitutive equations relative to the current reference.

$$\psi = \hat{\psi}(\mathbf{F}^{e-1}, \mathbf{g}, \mathbf{t}^e, \theta) = \rho_0^{-1} J^{e-1} \hat{\mathfrak{w}}(\bar{\mathbf{c}}^e(\mathbf{F}^{e-1}, \mathbf{g}), \bar{\mathbf{t}}(\mathbf{F}^{e-1}, \mathbf{t}^e), \theta), \tag{1.20}$$

$$\boldsymbol{\sigma} = 2\rho \frac{\partial \hat{\psi}}{\partial \mathbf{g}}\bigg|_{\mathbf{F}^{e-1}, \mathbf{t}^e, \theta}, \tag{1.21}$$

$$(\mathbf{j})^b_\alpha = (\mathbf{F}^e)^c_\alpha \left[-(\mathbf{g})_{cd} (\boldsymbol{\sigma})^{db} + \rho \hat{\psi}\, \delta^b_c + (\mathbf{t}^e)^a_{cd} (\boldsymbol{\sigma}^d)^{bd}_a \right], \tag{1.22}$$

$$\boldsymbol{\sigma}^d = 2\rho \frac{\partial \hat{\psi}}{\partial \mathbf{t}^e}\bigg|_{\mathbf{F}^{e-1}, \mathbf{g}, \theta}, \tag{1.23}$$

$$\eta = -\frac{\partial \hat{\psi}}{\partial \theta}\bigg|_{\mathbf{F}^{e-1}, \mathbf{g}, \mathbf{t}^e}. \tag{1.24}$$

The tensor $\tilde{\mathbf{j}}$ from (3.3.10) can be shown to be given by

$$\tilde{\mathbf{j}} = \rho \frac{\partial \hat{\psi}}{\partial \mathbf{F}^{c-1}}\bigg|_{\mathbf{g}, \mathbf{t}^e, \theta}. \tag{1.25}$$

The constitutive equations (1.21)-(1.25) can also be derived directly by considering the balance of energy (3.3.12) and the entropy production inequality (3.3.14) written relative to the current reference.

5.2 Noll-Wang's theory

Let us suppose that the plastic deformation $\mathbf{F}^p$ does not change with time, and consequently the crystal reference $\bar{\mathbb{K}}$ is given and should not be subject to variation (Noll-Wang's theory). This means, we are considering a simple body with frozen dislocations and the motion of this body is governed by Cauchy's equation of balance of macromomentum and moment of macromomentum alone. Restricting ourselves to isothermal processes, we assume also that the stored energy does not depend on the dislocation density $\bar{\mathbf{t}}$ [1]

$$W = W(\mathbf{F}, \mathbf{F}^p) = \hat{W}(\mathbf{F}^p, \mathbf{C}) = J^p \hat{\mathfrak{w}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C})). \tag{2.1}$$

[1] In engineering language we can say: the eigenenergy of dislocations is neglected in comparison with the stored energy due to the elastic deformation.

The principle of initial scaling indifference is still valid for $\hat{\mathfrak{w}}$, but, due to the absence of $\bar{\mathbf{t}}^e$ in the stored energy density, we have the following consequence

$$\mathbf{J} = \left.\frac{\partial W}{\partial \mathbf{F}^p}\right|_{\mathbf{F},\Theta} = \mathbf{F}^{p-T}(-\mathbf{F}^T\mathbf{g}\mathbf{P} + W\mathbf{1}). \tag{2.2}$$

In this model there are no balance equations for micromomentum and the driving force $\mathbf{J}$ need not be zero. However, in the absence of the body macroforce we can prove that

$$\mathrm{Div}\mathbf{J} = 0. \tag{2.3}$$

Indeed, applying the Div operator to $\mathbf{J}$ from (2.2) we get

$$(\mathbf{J})^A_{\alpha,A} = (\mathbf{F}^{p-T})^B_\alpha(-g_{ab}(\mathbf{P})^{aA}_{,A}(\mathbf{F})^b_B - g_{ab}(\mathbf{P})^{aA}(\mathbf{F})^b_{B,A} + W_{,B})$$
$$+(\mathbf{F}^{p-1})^B_{\alpha,A}(\mathbf{J})^A_\beta(\mathbf{F}^p)^\beta_B. \tag{2.4}$$

We calculate now the partial derivative of W according to (2.1)

$$W_{,B} = g_{ab}(\mathbf{P})^{aA}(\mathbf{F})^b_{A,B} + (\mathbf{J})^A_\alpha(\mathbf{F}^p)^\alpha_{A,B}. \tag{2.5}$$

Substituting (2.5) into (2.4) and taking the static equation (3.2.7) into account, one can see that (2.3) is valid. We denote by $\mathbf{B}$ the following tensor

$$\mathbf{B} = \mathbf{C}\mathbf{S} - W\mathbf{1}, \quad \mathbf{J} = -\mathbf{F}^{p-T}\mathbf{B}. \tag{2.6}$$

Then $\mathbf{B}$ satisfies the following equation

$$(\mathbf{B})^A_{B,A} + (\mathbf{B})^A_C(\mathbf{F}^p)^\alpha_B(\mathbf{F}^{p-1})^B_{\alpha,A} = 0. \tag{2.7}$$

From the balance of moment of momentum it follows that $\mathbf{B}$ is symmetric with respect to the tensor $\mathbf{C}$

$$\mathbf{B}\mathbf{C} = \mathbf{C}\mathbf{B}^T. \tag{2.8}$$

Eqs. (2.7), (2.8) were first obtained by Epstein & Maugin (1990).

5.3 Linearized theory

We assume again that the deformation fields $\mathbf{F}, \mathbf{F}^p, \mathbf{F}^e$ are given by (2.4.1). In this case the references $\mathbb{K}_0, \mathbb{K}_t$ and $\bar{\mathbb{K}}_t$ differ from each other by small

distorsions, so that they can be identified. Therefore, there is no need to distinguish between upper case, lower case and Greek indices. We also can choose the metric $\mathbf{g}$ to coincide with the identity map $\mathbf{1}$ and we can identify tangent and cotangent spaces. Thus, there is no need to distinguish between co- and contravariant tensors. All formulae obtained in Section 2.4 can now be applied. Especially we have the additive decomposition of the total (small) strain tensor into its elastic and plastic parts. The finite dislocation density measure $\mathbf{T}^p$ can be replaced by the linearized one given by (2.4.13). Restricting ourselves again to statics under the condition of constant temperature we can express the stored energy density per unit volume in the form

$$w = \hat{w}(\boldsymbol{\epsilon}^e, \boldsymbol{\alpha}) = \hat{w}(\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^p, \mathrm{curl}\boldsymbol{\beta}^p). \tag{3.1}$$

The equilibrium equations (3.4.4),(3.4.5) remain unchanged after linearization

$$\mathrm{div}\boldsymbol{\sigma} = \mathbf{0}, \tag{3.2}$$

$$\boldsymbol{\sigma}^T = \boldsymbol{\sigma}. \tag{3.3}$$

We show now how to linearized the equations (3.4.8), (3.4.9) and (3.4.10). Choosing the skew-symmetric microstress tensor $\mathbf{p}^d$ to satisfy the equation (3.4.9), we can introduce the following second rank tensor $\boldsymbol{\tau}$ with components

$$\tau_{ab} = -\frac{1}{2}\varepsilon_{bcd}(\mathbf{p}^d)_{acd}. \tag{3.4}$$

This tensor is uniquely defined by $\mathbf{p}^d$ due to the associate representation of skew-symmetric tensors. We also call $\boldsymbol{\tau}$ the couple stress tensor. Substituting $(\mathbf{p}^d)_{abc} = -\varepsilon_{dbc}\tau_{ad}$ into the equation (3.4.8) we have

$$\mathrm{curl}\boldsymbol{\tau} + \mathbf{j} = \mathbf{0}. \tag{3.5}$$

or in components

$$\varepsilon_{bcd}\tau_{ad,c} + j_{ab} = 0. \tag{3.5}$$

Linearizing (3.4.10) one can show that the driving force is approximated by the Cauchy stress taken with minus sign

$$\mathbf{j} = -\boldsymbol{\sigma}, \quad j_{ab} = -\sigma_{ab}. \tag{3.6}$$

Therefore, the balance of micromomentum (3.5) reduces to

$$\mathrm{curl}\boldsymbol{\tau} - \boldsymbol{\sigma} = \mathbf{0}. \tag{3.7}$$

According to (3.1) we have the following constitutive equations

$$\boldsymbol{\sigma} = \frac{\partial \hat{w}}{\partial \boldsymbol{\epsilon}^e} = \frac{\partial \hat{w}}{\partial \boldsymbol{\epsilon}}. \tag{3.8}$$

$$\boldsymbol{\tau} = \frac{\partial \hat{w}}{\partial \boldsymbol{\alpha}}. \tag{3.9}$$

The linearized driving force tensor is given by

$$\mathbf{j} = -\boldsymbol{\sigma} = \frac{\partial \hat{w}}{\partial \boldsymbol{\epsilon}^p}. \tag{3.10}$$

The linearized equations (3.2), (3.3) and (3.7) are not identical with those postulated by Kröner. In Kröner's theory the equations corresponding to (3.2) and (3.7) can be written in our notation as follows (see Kröner, 1980, Eqs. (41),(42))

$$\sigma_{ij,j} = 0, \tag{3.11}$$

$$\tau_{ij,j} - \varepsilon_{ijk}\sigma_{jk} = 0, \tag{3.12}$$

with σ_{ij} denoting an unsymmetric stress tensor. The existence of the unsymmetric stress tensor is due to the fact that Kröner did not postulate any balance law for the moment of macromomentum, or equivalently saying, his energy density is assumed as a function of $\boldsymbol{\beta}^e$ and $\boldsymbol{\alpha}$ (see Kröner, 1980, formula (40)). Eliminating the skew-symmetric part of $\boldsymbol{\beta}^e$ in his energy density and applying the principle of virtual work, one can derive the equations identical with (3.2), (3.3) and (3.7). It is also worth noting that in his applications to concrete problems Kröner always used the symmetric stress tensor satisfying the equilibrium equations (3.2) and (3.3).

Since the elastic strain and the dislocation density are small, we can approximate the stored energy density by a quadratic form of $\boldsymbol{\epsilon}^e$ and $\boldsymbol{\alpha}$

$$w = \frac{1}{2}C_{abcd}(\boldsymbol{\epsilon}^e)_{ab}(\boldsymbol{\epsilon}^e)_{cd} + \frac{1}{2}A_{abcd}(\boldsymbol{\alpha})_{ab}(\boldsymbol{\alpha})_{cd}. \tag{3.13}$$

In (3.13) we assume explicitly that there is no cross-term between $\boldsymbol{\epsilon}^e$ and $\boldsymbol{\alpha}$. The constants C_{abcd} and A_{abcd} should satisfy the following symmetry properties

$$C_{abcd} = C_{bacd} = C_{abdc} = C_{cdab}, \tag{3.14}$$

and

$$A_{abcd} = A_{cdab}. \tag{3.15}$$

Eqs. (3.14) and (3.15) reduce the number of independent constants from 81 to 21 for C_{abcd} and to 45 for A_{abcd} in the general case of anisotropy. A further reduction is possible for special types of crystal symmetry.

According to (3.13) the stress and couple stress tensors are given by

$$\sigma_{ab} = C_{abcd}(\epsilon^e)_{cd}, \tag{3.16}$$

$$\tau_{ab} = A_{abcd}(\alpha)_{cd}. \tag{3.17}$$

Due to (3.16) one can determine first the stress field inside the body, provided the dislocation density $\boldsymbol{\alpha}$ is prescribed. Following Kröner, we introduce the tensor field of stress functions $\boldsymbol{\chi}$ such that

$$\boldsymbol{\sigma} = \mathrm{inc}\boldsymbol{\chi}. \tag{3.18}$$

It is easy to prove the identities

$$\mathrm{div}\,\mathrm{inc} \equiv 0, \quad \mathrm{inc}\,\mathrm{def} \equiv 0, \tag{3.19}$$

which are similar to those classical formulae with div, grad and curl in vector analysis (see Kröner 1958,1980). Therefore the stress field given by (3.17) satisfies the equilibrium equation (3.2) and (3.3) identically. Now using Hooke's law (3.15) to express $\boldsymbol{\epsilon}^e$ through $\boldsymbol{\sigma}$ and then through the tensor field $\boldsymbol{\chi}$ via (3.17), we can substitute the result into the incompatibility equation (2.4.18) to derive the field equations for $\boldsymbol{\chi}$. The latter can be solved for many special problems (Kröner 1958,1980).

5.4 Link to the macroscopic elastoplasticity

It is more difficult to see the link of the theory proposed in this paper with the macroscopic elastoplasticity (cf. Lee 1969 and a cycle of our works Stumpf & Badur 1990; Stumpf 1993; Le & Stumpf 1993*a*; Schieck & Stumpf 1993,1994). First of all we should point out the striking difference between the constitutive equations of these two theories: while the former is reversible, the latter is not. There are two possible ways of making them connected. The first way is associated with an assumption of non-convexity of the stored energy leading to the co-existence of phases and the formation of microstructure (see, for example, Ericksen 1975; Ball & James 1987; Knowles 1991). The dissipation is then defined as the rate of work

done by the Eshelby driving force acting on moving interphases. In the case of 1-D elasticity Knowles has shown that a nucleation criterion and a kinetic law are needed to make the problem well-posed. This way is very attractive and promising but not yet finished. The second way is direct. We assume again that the free energy density per unit crystal volume does not depend on the dislocation density so that

$$\Psi = \hat{\Psi}(\mathbf{F}^p, \mathbf{C}, \Theta) = \rho_0^{-1} J^p \hat{\mathfrak{w}}(\bar{\mathbf{c}}^e(\mathbf{F}^p, \mathbf{C}), \Theta). \tag{4.1}$$

In constrast to Noll-Wang's theory, here the plastic deformation can change with time. However it cannot be varied in an arbitrary manner, but should be subject to some anholonomic constraint. We introduce the tensor field $\bar{\mathbf{k}}$ as follows

$$\bar{\mathbf{k}} = \mathbf{g}^{-1}\bar{\mathbf{c}}^e\bar{\mathbf{s}} - \hat{\mathfrak{w}}\mathbf{g}^{-1}. \tag{4.2}$$

We call $\bar{\mathbf{k}}$ the plastic stress tensor (Le & Stumpf 1993*a*). Note that $\bar{\mathbf{k}}$ is symmetric, what is the consequence of the symmetry of $\mathbf{B}$ with respect to $\mathbf{C}$ (see Section 5.2). As an example of constraint we can propose the following: the plastic deformation rate $\bar{\mathbf{d}}^p$ is zero as long as the plastic stress tensor $\bar{\mathbf{k}}$ is inside a convex yield surface

$$f(\bar{\mathbf{k}}) < 0 \Rightarrow \bar{\mathbf{d}}^p = \mathbf{0}, \tag{4.3}$$

Due to the constraint (4.3), the plastic deformation cannot be varied arbitrarily as long as the plastic stress tensor is inside the yield surface, and Cauchy's balance of macromomentum and moment of macromomentum alone governs the motion of the body. The microstress and couple stress tensors vanish. Therefore the entropy production inequality relative to the initial reference takes the form (Le & Stumpf 1993*a*)

$$\rho_0(N\dot{\Theta} + \dot{\Psi}) - < \mathbf{gP}, \dot{\mathbf{F}} > + < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} > \leq 0. \tag{4.4}$$

Taking the time derivative of Ψ given by (4.1) we have

$$\dot{\Psi} = < \frac{\partial \Psi}{\partial \mathbf{F}^p}, \dot{\mathbf{F}}^p > + < \frac{\partial \Psi}{\partial \mathbf{F}}, \dot{\mathbf{F}} > + \frac{\partial \hat{\Psi}}{\partial \Theta}\dot{\Theta}. \tag{4.5}$$

Substituting (4.5) into (4.4), we can transform (4.4) to (see Le & Stumpf 1993*a*)

$$< (\rho_0 \frac{\partial \Psi}{\partial \mathbf{F}} - \mathbf{gP}), \dot{\mathbf{F}} > + \rho_0(N + \frac{\partial \Psi}{\partial \Theta})\dot{\Theta}$$

$$- < \frac{\partial \Psi}{\partial \mathbf{F}^p}, \dot{\mathbf{F}}^p > + < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} > \leq 0. \tag{4.6}$$

A procedure similar to that presented in Section 5.1 leads to the constitutive equations

$$\mathbf{P} = \rho_0 \mathbf{g}^{-1} \frac{\partial \Psi}{\partial \mathbf{F}}\bigg|_{\mathbf{F}^p, \Theta}, \tag{4.7}$$

$$N = - \frac{\partial \Psi}{\partial \Theta}\bigg|_{\mathbf{F}, \mathbf{F}^p}. \tag{4.8}$$

Due to (4.1) the constitutive equation (4.8) can be rewritten also as follows

$$\mathbf{S} = 2\rho_0 \frac{\partial \hat{\Psi}}{\partial \mathbf{C}}\bigg|_{\mathbf{F}^p, \Theta}. \tag{4.9}$$

The inequality (4.4) reduces to the dissipation inequality

$$< \mathbf{J}, \dot{\mathbf{F}}^p > + < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} > \leq 0, \tag{4.10}$$

where

$$\mathbf{J} = \rho_0 \frac{\partial \hat{\Psi}}{\partial \mathbf{F}^p}\bigg|_{\mathbf{C}, \Theta} = \mathbf{F}^{p-T}(-\mathbf{C}\mathbf{S} + \rho_0 \Psi \mathbf{1}). \tag{4.11}$$

Multiplying (4.10) by J^{p-1} we can transform it to the dissipation inequality relative to the crystal reference (Le & Stumpf 1993*a*)

$$- < \bar{\mathbf{k}}, \bar{\mathbf{d}}^p > + < \frac{\mathrm{grad}_{\bar{\mathbf{K}}_t} \bar{\theta}}{\bar{\theta}}, \bar{\mathbf{q}} > \leq 0. \tag{4.12}$$

We show the derivation of (4.12) directly in components. Multiplying the first term on the right-hand side of (4.10) by J^{p-1} and recalling (4.11), we get

$$J^{p-1} < \mathbf{J}, \dot{\mathbf{F}}^p > = J^{p-1} (\mathbf{F}^{p-1})^B_\alpha [-(\mathbf{C})_{BC} (\mathbf{S})^{CA} + \rho_0 \hat{\Psi} \delta^A_B] (\dot{\mathbf{F}}^p)^\alpha_A. \tag{4.13}$$

Replacing $\mathbf{C}$, $\mathbf{S}$ and $\rho_0 \hat{\Psi}$ by $\bar{\mathbf{c}}$, $\bar{\mathbf{s}}$ and $\hat{\mathfrak{w}}$ according to (1.5.7), (3.2.12) and (4.1), respectively, we can transform (4.13) in the following way

$$J^{p-1} < \mathbf{J}, \dot{\mathbf{F}}^p > = [-(\bar{\mathbf{c}}^e)_{\alpha\gamma} (\bar{\mathbf{s}})^{\gamma\beta} + \hat{\mathfrak{w}} \delta^\beta_\alpha] (\bar{\mathbf{l}}^p)^\alpha_\beta. \tag{4.14}$$

where $\bar{\mathbf{l}}^p = \dot{\mathbf{F}}^p \mathbf{F}^{p-1}$. Raising the index α of the tensor in the brackets and lowering the same index of $\bar{\mathbf{l}}^p$ with the help of $\mathbf{g}$ and using the symmetry of $\bar{\mathbf{k}}$ as well as the definition (1.6.9), we obtain

$$J^{p-1} < \mathbf{J}, \dot{\mathbf{F}}^p > = - < \bar{\mathbf{k}}, \bar{\mathbf{d}}^p > . \tag{4.15}$$

In order to transform the second term on the right-hand side of (4.10) we recall that

$$(\mathbf{Q})^A = J^p(\mathbf{F}^{p-1})^A_\alpha(\bar{\mathbf{q}})^\alpha, \quad \Theta = \bar{\theta}. \tag{4.16}$$

Substitution of (4.16) into the second term of (4.10) followed by the multiplication by J^{p-1} gives

$$J^{p-1} < \frac{\mathrm{Grad}\Theta}{\Theta}, \mathbf{Q} >= \frac{1}{\bar{\theta}}\bar{\theta}_{,A}(\mathbf{F}^{p-1})^A_\alpha(\bar{\mathbf{q}})^\alpha = \frac{\bar{\theta}_{,\alpha}}{\bar{\theta}}(\bar{\mathbf{q}})^\alpha. \tag{4.17}$$

In the last step of (4.17) the definition of the relative derivative (1.3.2) was used. Combination of (4.15) and (4.17) leads to (4.12)

Let us assume that there is no coupling between heat exchange and plastic flow, and let $-\mathrm{grad}_{\bar{\mathbb{K}}_t}\bar{\theta}/\bar{\theta}$ be denoted by $\bar{\mathbf{f}}$. Then we formulate the generalized normality rule or, equivalently, the principle of maximum dissipation rate (von Mises 1928; Hill 1948; Drucker 1951; Ziegler 1958) relative to the crystal reference in the form

$$\bar{\mathbf{k}} = \partial_{\bar{\mathbf{d}}^p}\bar{\mathcal{D}}^p, \quad \bar{\mathbf{f}} = \nu\partial_{\bar{\mathbf{q}}}\bar{\mathcal{D}}^h, \quad \nu = \bar{\mathcal{D}}^h(\partial_{\bar{\mathbf{q}}}\bar{\mathcal{D}}^h\cdot\bar{\mathbf{q}})^{-1}, \tag{4.18}$$

with

$$\bar{\mathcal{D}}^p = \bar{\mathcal{D}}^p(\bar{\mathbf{d}}^p, \bar{\theta}) \geq 0, \quad \bar{\mathcal{D}}^h = \bar{\mathcal{D}}^h(\bar{\mathbf{q}}, \bar{\theta}) \geq 0. \tag{4.19}$$

The dissipation functions $\bar{\mathcal{D}}^p$ and $\bar{\mathcal{D}}^h$ are supposed to be positive definite, convex and lower-semi-continuous with respect to their arguments $\bar{\mathbf{d}}^p$ and $\bar{\mathbf{q}}$, respectively. The symbol ∂ is used to denote the sub-differential of convex functions (Moreau 1970, consult also Maugin 1992, Appendix 2). An example of the dissipation functions can be given for the case of isotropic materials with a generalization of von Mises' and Fourier's laws referred to the crystal reference

$$\bar{\mathcal{D}}^p(\bar{\mathbf{d}}^p, \bar{\theta}) = \begin{cases} \sigma_0(2/3)^{1/2}[g^{\alpha\gamma}g^{\beta\delta}\bar{d}^p_{\alpha\beta}\bar{d}^p_{\gamma\delta}]^{1/2}: & \bar{g}^{\alpha\beta}\bar{d}^p_{\alpha\beta} = 0 \\ +\infty: & \text{otherwise} \end{cases} \tag{4.20}$$

$$\bar{\mathcal{D}}^h(\bar{\mathbf{q}}, \bar{\theta}) = \frac{1}{\kappa\bar{\theta}}g_{\alpha\beta}\bar{q}^\alpha\bar{q}^\beta. \tag{4.21}$$

Here σ_0 is the yield stress in uniaxial tension experiment and κ the thermal conductivity. From (4.21) it follows that $\nu = 1/2$ and $(4.18)_2$ reduces to Fourier's equation

$$\bar{\mathbf{q}} = -\kappa\mathrm{grad}_{\bar{\mathbb{K}}_t}\bar{\theta}. \tag{4.22}$$

Further, it is convenient (but not necessary) to suppose that no volume change occurs in the plastic flow so that

$$\bar{\rho} = \rho_0, \quad \mathrm{tr}(\mathbf{g}^{-1}\bar{\mathbf{d}}^p) = 0. \tag{4.23}$$

This condition excludes automatically the case, in which the dissipation function of (4.19) is equal to infinity. Note that while $\bar{\mathcal{D}}^h$ is a quadratic form of $\bar{\mathbf{q}}$ (Onsager's principle), $\bar{\mathcal{D}}^p$ is only a homogeneous function of first degree with respect to $\bar{\mathbf{d}}^p$. This can be explained by comparing the mechanism of heat exchange with the nature of plastic flow. In the latter case a certain amount of the plastic stress tensor (dissipative) should be reached to initiate the plastic flow (similar to the mechanism of dry friction). This is in agreement with our constraint (4.3). From the other side it can be shown that the equation $(4.18)_1$ is equivalent to the conventional yield condition (4.3) (with the convex yield surface) and the associated flow rule if and only if the dissipation function is homogeneous of first degree with respect to $\bar{\mathbf{d}}^p$. The equation $(4.18)_1$ then establishes the (nonsingle-valued) connection between $\bar{\mathbf{k}}$ and $\bar{\mathbf{d}}^p$. However, it is worthwhile to emphasize that the dissipation itself is uniquely determined by $\bar{\mathbf{d}}^p$. To rewrite $(4.18)_1$ in a more usual form, we apply the Fenchel transformation (Moreau 1970) to the dissipation function $\bar{\mathcal{D}}^p$ to obtain the so-called plastic potential $\bar{\varphi}(\bar{\mathbf{k}}, \bar{\theta})$. Then the constitutive equation $(4.18)_1$ is equivalent to the flow rule

$$\bar{\mathbf{d}}^p = \partial_{\bar{\mathbf{k}}}\bar{\varphi}(\bar{\mathbf{k}}, \bar{\theta}). \tag{4.24}$$

For the dissipation function (4.19) the plastic potential has the form

$$\bar{\varphi} = \begin{cases} 0: & [(g_{\alpha\gamma}g_{\beta\delta} - \frac{1}{3}g_{\alpha\beta}g_{\gamma\delta})\bar{k}^{\alpha\beta}\bar{k}^{\gamma\delta}]^{1/2} \leq \sigma_0(2/3)^{1/2} \\ +\infty: & \text{otherwise} \end{cases} \tag{4.25}$$

Eqs. (4.18) and (4.24) and their equivalent versions in the initial and current description were first obtained in our paper (Le & Stumpf 1993*a*).

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