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A Cosserat theory for elastoviscoplastic single crystals at finite deformation

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IN THIS WORK, displacement and lattice rotation are regarded as independent degrees of freedom. They are connected only on the constitutive level and by the balance equations. The description of plastic deformation is based on the slip theory. Elastic lattice curvature and torsion are associated with couple-stresses. The continuum theory of dislocations has been revisited to derive the kinematics of plastic lattice torsion-curvature. Explicit constitutive equations and hardening rules are proposed to close the theory in the case of elastoviscoplasticity. The thermodynamical formulation of the model involves internal variables which are similar to the densities of statistically stored dislocations and the densities of geometrically necessary dislocations. Accordingly, the proposed Cosserat theory can be regarded, on the one hand, as the classical crystal plasticity theory complemented by lattice curvature and torsion variables and, on the other hand, as the continuum theory of dislocations closed by the missing hardening variables and constitutive equations within the appropriate micropolar framework. A generalization of Mandel's elastoviscoplastic decomposition of strain is used especially for the torsion-curvature measure at finite deformation.

1. Introduction

MANDEL [1] introduced the notion of oriented microelements characterized by some hidden directors into the theory of elastoviscoplasticity. The epoch-making expression "trièdre directeur" is directly taken from the Cosserat brothers' well-known work [2]. The relative rotation of neighbouring microelements may induce local couple stresses. To the first approximation Mandel neglects them and regards the single crystal and the polycrystal as a classical continuum. We propose here the strict treatment of the single crystal as a Cosserat continuum.

NYE [3] noticed that after bending or torsion, a crystal contains excess dislocations of a definite sign that give rise to lattice curvature. In a modelling of single crystals with more reference to dislocations, this additional deformation possibility should be taken into account. Furthermore KRÖNER [4] claimed that the macroscopic response of a medium to lattice curvature is the existence of actual Cosserat couple stresses. The couple-stresses may have the same order of magnitude as force-stresses under some circumstances [5, 6]. In these early works Kröner regards the dislocated crystal as a Cosserat medium. However, his theory deals with symmetric force-stresses and he suggests later that there may be fundamental differences between the dislocation theory and the Cosserat theory [7].

The reason for such a misunderstanding stems from the frequent use in literature of the Cosserat continuum as the medium in which single dislocations may be

embedded. KESSEL [8] computes the force and couple stress fields around screw and edge dislocations in a Cosserat continuum. In the present work we claim that the continuum containing a large number of dislocations in the sense of the continuum theory of dislocations [3], can be modelled as a Cosserat continuum. KRÖNER [9] argues that the rotation of the crystal lattice with dislocations is not the eigenrotation of physical particles but the rotation of a structure. This pleads against the constrained Cosserat theory that is usually used in the continuum theory of dislocations (see Sec. 3.4). As a result, in the Cosserat theory presented here, the rotational degrees of freedom are independent of the displacement field and are linked only on the constitutive level and by the balance equations. While the definition of the Cosserat directors involved in the continuum theory of dislocation is generally left unspecified, the "trièdre directeur" in this work is clearly made of three orthogonal lattice vectors attached to each volume element in a released state of the crystal element. As for them, CLAUS and ERINGEN [10] also erect a lattice triad at every point of the continuum. A most interesting point in their work is that they resort to a micromorphic continuum. They also propose a phenomenological treatment of micromorphic elastoplasticity but they do not derive the crystallographic expressions of plastic slip and curvature nor the necessary constitutive equations. WOŹNIAK [11, 12] devoted great attention to the structural interpretation of the additional degrees of freedom of the micromorphic continuum and considered also bodies with lattice structure. More recently, LE and STUMPF [13, 14] have reformulated the continuum theory of dislocations in the modern language of differential geometry and they also resort to an oriented continuum. In order to get a closed formulation of our model including constitutive equations, we will focus on the Cosserat continuum.

The characteristic size of the volume element must be large enough so that it contains a large number of dislocations and that a mean crystal orientation can be unambiguously defined at each time. It will finally depend on the structural application one aims at.

In Secs. 2.1 to 2.3, the main features of the Cosserat theory at finite deformation are recalled in order to introduce the subsequent developments in elastoviscoplasticity. The evolution rule for plastic curvature is derived from the continuum theory of dislocations in Sec. 3.3, after recalling the closure problem of the continuum theory of dislocations. Explicit constitutive equations are then proposed to solve this problem in Sec. 4. The notations and some classical results used throughout this article are explained in the Appendix.

2. A Cosserat theory for single crystals

2.1. Kinematics of the Cosserat continuum

A material point $M \in \mathcal{B}$ at time t_0 is described by its position $\underline{\mathbf{X}}$ and its inner state, for an arbitrary initial placement, chosen as the reference site. At time t, its position is $\underline{\mathbf{x}}(\underline{\mathbf{X}}, t)$ and its inner state $\underset{\sim}{\mathbf{R}}(\underline{\mathbf{X}}, t)$, in a given reference frame E. If

$(\underline{\mathbf{d}}_i)_{i=1,3}$ are three orthogonal lattice vectors in a released state at t and $(\underline{\mathbf{d}}_i^0)_{i=1,3}$ their initial placement in E, then the rotation $\underline{\underline{\mathbf{R}}}$ is defined through

$$\underline{\mathbf{d}}_i = \underline{\underline{\mathbf{R}}}\, \underline{\mathbf{d}}_i^0 \tag{2.1}$$

with

$$\underline{\underline{\mathbf{R}}}\, \underline{\underline{\mathbf{R}}}^T = \underline{\underline{\mathbf{1}}}, \qquad \underline{\underline{\mathbf{R}}}(\underline{\mathbf{X}}, t_0) = \underline{\underline{\mathbf{1}}} \qquad \text{and} \qquad \operatorname{Det} \underline{\underline{\mathbf{R}}} = 1. \tag{2.2}$$

A rotating frame $E^\sharp(M)$ is attached to the lattice structure at each point $M \in \mathcal{B}$ and each vector and tensor variable y considered with respect to $E^\sharp$ will be denoted by ${}^\sharp y$.

The rotation field $\underline{\underline{\mathbf{R}}}(\underline{\mathbf{X}}, t)$ can be replaced by the vector field $\underline{\mathbf{\Phi}}(\underline{\mathbf{X}}, t)$ given by Eq. (A.12) of the Appendix. The three components of $\underline{\mathbf{\Phi}}$ are three degrees of freedom of the continuum, in addition to the three components of the displacement field

$$\underline{\mathbf{u}}(\underline{\mathbf{X}}, t) = \underline{\mathbf{x}}(\underline{\mathbf{X}}, t) - \underline{\mathbf{X}}. \tag{2.3}$$

Here, $\underline{\mathbf{u}}$ and $\underline{\mathbf{\Phi}}$ are regarded as independent kinematic variables which can be connected on the balance or constitutive level or by some constraint.

The deformation gradient classically links the current infinitesimal material segment $d\underline{\mathbf{x}}$ with its initial position $d\underline{\mathbf{X}}$

$$d\underline{\mathbf{x}} = \underline{\underline{\mathbf{F}}}\, d\underline{\mathbf{X}} \tag{2.4}$$

so that

$$\underline{\underline{\mathbf{F}}} = \underline{\mathbf{u}} \otimes \underline{\nabla} = u_{i,j}\, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \tag{2.5}$$

(in the absence of other indication, partial derivatives are taken with respect to the X_j).

Similarly, we compute the variation $d\underline{\underline{\mathbf{R}}}$ of microrotation along a material segment $d\underline{\mathbf{X}}$. Defining $\delta\, \underline{\mathbf{\Phi}}$ by

$$(d\underline{\underline{\mathbf{R}}})\, \underline{\underline{\mathbf{R}}}^T = \underline{\underline{\mathbf{1}}} \times \delta\underline{\mathbf{\Phi}} = \underline{\underline{\underline{\epsilon}}}\, \delta\, \underline{\mathbf{\Phi}} \tag{2.6}$$

we derive

$$\delta\, \underline{\mathbf{\Phi}} = -\frac{1}{2}\, \underline{\underline{\underline{\epsilon}}}\, (d\underline{\underline{\mathbf{R}}}\, \underline{\underline{\mathbf{R}}}^T) = \underline{\underline{\mathbf{\Gamma}}}\, d\underline{\mathbf{X}} \tag{2.7}$$

with

$$\underline{\underline{\mathbf{\Gamma}}} = \frac{1}{2}\, \underline{\underline{\underline{\epsilon}}} : (\underline{\underline{\mathbf{R}}}\, (\underline{\underline{\mathbf{R}}}^T \otimes \underline{\nabla})). \tag{2.8}$$

The notation $\delta \underline{\Phi}$ means that $\delta \underline{\Phi}$ is not a total differential, as can be seen from (2.7). Contrary to $\underset{\sim}{\mathbf{F}}$, $\underset{\sim}{\Gamma}$ generally is not invertible. With respect to the local space frame $E^\sharp$,

$$(2.9) \qquad {}^\sharp d\underline{x} = {}^\sharp\underset{\sim}{\mathbf{F}}\, d\underline{X} \qquad \text{and} \qquad {}^\sharp\delta\underline{\Phi} = {}^\sharp\underset{\sim}{\Gamma}\, d\underline{X},$$

where ${}^\sharp d\underline{x} = \underset{\sim}{\mathbf{R}}^T\, d\underline{x}$ and ${}^\sharp\delta\underline{\Phi} = \underset{\sim}{\mathbf{R}}^T\, \delta\underline{\Phi}$, and

$$(2.10) \qquad {}^\sharp\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{R}}^T\, \underset{\sim}{\mathbf{F}}, \qquad {}^\sharp\underset{\sim}{\Gamma} = \underset{\sim}{\mathbf{R}}^T\, \underset{\sim}{\Gamma}.$$

It can be seen that the relative measures ${}^\sharp\underset{\sim}{\mathbf{F}}$ and ${}^\sharp\underset{\sim}{\Gamma}$ are invariant under any Euclidean transformation [15]. Accordingly they are natural Cosserat strains for the development of constitutive equations. They are called respectively the Cosserat deformation tensor and the wryness (or bend-twist, or torsion-curvature) tensor. An alternative expression of the wryness tensor is then

$$(2.11) \qquad {}^\sharp\underset{\sim}{\Gamma} = -\frac{1}{2}\underline{\underline{\epsilon}} : (\underset{\sim}{\mathbf{R}}^T\, (\underset{\sim}{\mathbf{R}} \otimes \underline{\nabla})).$$

One defines next the velocity and the gyration tensor

$$(2.12) \qquad \underline{\mathbf{v}} = \dot{\underline{\mathbf{u}}} = \dot{u}_i\, \underline{\mathbf{e}}_i \qquad \text{and} \qquad \underset{\sim}{\boldsymbol{\upsilon}} = \dot{\underset{\sim}{\mathbf{R}}}\, \underset{\sim}{\mathbf{R}}^T$$

which can be replaced by the associated gyration vector

$$(2.13) \qquad \overset{\times}{\underline{\boldsymbol{\upsilon}}} = -\frac{1}{2}\underline{\underline{\epsilon}}\, \underset{\sim}{\boldsymbol{\upsilon}}$$

since it is skew-symmetric. The time derivative of the Cosserat strains can be related to the gradient of the latter quantities:

$$(2.14) \qquad {}^\sharp\dot{\underset{\sim}{\mathbf{F}}}\, {}^\sharp\underset{\sim}{\mathbf{F}}^{-1} = \underset{\sim}{\mathbf{R}}^T\, (\underline{\mathbf{v}} \otimes \underline{\nabla}^c - \underline{\mathbf{1}} \times \overset{\times}{\underline{\boldsymbol{\upsilon}}})\, \underset{\sim}{\mathbf{R}},$$

$$(2.15) \qquad {}^\sharp\dot{\underset{\sim}{\Gamma}}\, {}^\sharp\underset{\sim}{\mathbf{F}}^{-1} = \underset{\sim}{\mathbf{R}}^T\, \overset{\times}{\underline{\boldsymbol{\upsilon}}} \otimes \underline{\nabla}^c\, \underset{\sim}{\mathbf{R}},$$

where $\underline{\nabla}^c = \dfrac{\partial}{\partial x_i}\, \underline{\mathbf{e}}_i = \underset{\sim}{\mathbf{F}}^{-T}\, \underline{\nabla}$ (Euclidean representation, c stands for current).

$\underline{\mathbf{v}} \otimes \underline{\nabla}^c - \underset{\sim}{\boldsymbol{\upsilon}}$ is the relative velocity gradient and describes the local motion of the material element with respect to the microstructure.

2.2. Forces and stresses

In order to introduce forces and stresses and to deduce the equilibrium equations, we resort to the method of virtual power developed by GERMAIN [16] in the case of micromorphic media. The method is readily adapted to the case of a Cosserat continuum.

The virtual motions are the velocity $\underline{\mathbf{v}}$ and the gyration $\overset{\times}{\underline{\boldsymbol{\upsilon}}}$ (or microrotation rate vector). The next step is to choose the form of the virtual power of a system of forces. Within the framework of a first gradient theory, the virtual power of the internal forces is a linear form of the virtual motions and their gradients. The principle of material frame indifference requires that this linear form should be invariant under any Euclidean transformation. That is why we will work with the objective quantities $\underline{\mathbf{v}} \otimes \underline{\nabla}^c - \underset{\sim}{\upsilon}$ and $\overset{\times}{\underline{\boldsymbol{\upsilon}}} \otimes \underline{\nabla}^c$. The dual quantities involved in the linear form of the virtual power of the internal forces are denoted $\underset{\sim}{\boldsymbol{\sigma}}$ and $\underset{\sim}{\boldsymbol{\mu}}$ respectively, and are assumed to be objective tensors. For objectivity reasons the dual variable associated with $\underline{\mathbf{v}}$ is zero. For any subdomain $\mathcal{D} \subset \mathcal{B}$

$$\begin{aligned}
\mathcal{P}_{(i)} &= -\int_{\mathcal{D}} \left(\underset{\sim}{\boldsymbol{\sigma}} : (\underline{\mathbf{v}} \otimes \underline{\nabla}^c - \underset{\sim}{\upsilon}) + \underset{\sim}{\boldsymbol{\mu}} : (\overset{\times}{\underline{\boldsymbol{\upsilon}}} \otimes \underline{\nabla}^c) \right) dV \\
&= -\int_{\mathcal{D}} \left(\sigma_{ij}\, v_{i,j} + \mu_{ij}\, \overset{\times}{v}_{i,j} - \sigma_{ij}\, v_{ij} \right) dV \\
&= -\int_{\mathcal{D}} \left(\sigma_{ij}\, v_i + \mu_{ij}\, \overset{\times}{v}_i \right)_{,j} dV + \int_{\mathcal{D}} \left(\sigma_{ij,j}\, v_i + (\mu_{ij,j} - \epsilon_{ikl}\, \sigma_{kl}) \overset{\times}{v}_i \right) dV ,
\end{aligned}$$

that is

$$\mathcal{P}_{(i)} = -\int_{\partial\mathcal{D}} \left(\underline{\mathbf{v}}\, \underset{\sim}{\boldsymbol{\sigma}} + \overset{\times}{\underline{\boldsymbol{\upsilon}}}\, \underset{\sim}{\boldsymbol{\mu}} \right) . \underline{\mathbf{n}}\, dS + \int_{\mathcal{D}} \left(\underline{\mathbf{v}} . \underline{\operatorname{div}}\, \underset{\sim}{\boldsymbol{\sigma}} + \overset{\times}{\underline{\boldsymbol{\upsilon}}} . (\underline{\operatorname{div}}\, \underset{\sim}{\boldsymbol{\mu}} + 2\, \overset{\times}{\underline{\boldsymbol{\sigma}}}) \right) dV \tag{2.16}$$

(in this subsection the partial derivatives are taken with respect to the current configuration). The virtual power of external forces reads

$$\mathcal{P}_{(e)} = \int_{\mathcal{D}} \left(\underline{\mathbf{f}} . \underline{\mathbf{v}} + \underline{\mathbf{c}} . \overset{\times}{\underline{\boldsymbol{\upsilon}}} \right) dS. \tag{2.17}$$

The virtual power of contact forces must then be defined

$$\mathcal{P}_{(c)} = \int_{\partial\mathcal{D}} \left(\underline{\mathbf{t}} . \underline{\mathbf{v}} + \underline{\mathbf{m}} . \overset{\times}{\underline{\boldsymbol{\upsilon}}} \right) dS. \tag{2.18}$$

The dual quantities of the velocity and microrotation rate in $\mathcal{P}_{(e)}$ and $\mathcal{P}_{(c)}$ have the dimensions of volume or surface force and moment, respectively. The principle of virtual power then states that

$$\forall\, \mathcal{D} \subset \mathcal{B}, \quad \forall\, (\underline{\mathbf{v}}, \overset{\times}{\underline{\boldsymbol{\upsilon}}}) \quad \mathcal{P}_{(i)} + \mathcal{P}_{(e)} + \mathcal{P}_{(c)} = 0.$$

In particular

$$\forall\, \mathcal{D} \subset \mathcal{B}, \quad \forall\, (\underline{\mathbf{v}}, \overset{\times}{\underline{\boldsymbol{\upsilon}}}) \,/\, \underline{\mathbf{v}} = \overset{\times}{\underline{\boldsymbol{\upsilon}}} = 0 \quad \text{on } \partial\mathcal{D},$$

$$\int_{\mathcal{D}} \left(\underline{\mathbf{v}} . (\underline{\operatorname{div}}\, \underset{\sim}{\boldsymbol{\sigma}} + \underline{\mathbf{f}}) + \overset{\times}{\underline{\boldsymbol{\upsilon}}} . (\underline{\operatorname{div}}\, \underset{\sim}{\boldsymbol{\mu}} + 2\, \overset{\times}{\underline{\boldsymbol{\sigma}}} + \underline{\mathbf{c}}) \right) dV = 0.$$

Assuming that the quantities are continuous on $\mathcal{B}$, the local equilibrium equations follow

$$\begin{aligned} \underline{\operatorname{div}}\, \underset{\sim}{\boldsymbol{\sigma}} + \underline{\mathbf{f}} &= 0\,, \\ \underline{\operatorname{div}}\, \underset{\sim}{\boldsymbol{\mu}} + 2\,\overset{\times}{\underline{\boldsymbol{\sigma}}} + \underline{\mathbf{c}} &= 0. \end{aligned} \tag{2.19}$$

As a result, the principle of virtual power becomes

$$\forall\, \mathcal{D} \subset \mathcal{B}, \quad \forall\, (\underline{\mathbf{v}}, \overset{\times}{\underline{\boldsymbol{\upsilon}}}) \quad \int_{\partial \mathcal{D}} \left((\underset{\sim}{\boldsymbol{\sigma}}\, \underline{\mathbf{n}} - \underline{\mathbf{t}}) \,.\, \underline{\mathbf{v}} + (\underset{\sim}{\boldsymbol{\mu}}\, \underline{\mathbf{n}} - \underline{\mathbf{m}}) \,.\, \overset{\times}{\underline{\boldsymbol{\upsilon}}} \right) dV = 0,$$

from which the boundary conditions are deduced

$$\begin{aligned} \underset{\sim}{\boldsymbol{\sigma}}\, \underline{\mathbf{n}} &= \underline{\mathbf{t}}\,, \\ \underset{\sim}{\boldsymbol{\mu}}\, \underline{\mathbf{n}} &= \underline{\mathbf{m}}\,. \end{aligned} \tag{2.20}$$

$\underset{\sim}{\boldsymbol{\sigma}}$ is called the Cauchy force stress tensor and $\underset{\sim}{\boldsymbol{\mu}}$ the couple-stress tensor. They are generally not symmetric. A detailed account of Cosserat statics and dynamics can be found in [17].

2.3. Hyperelasticity

2.3.1. Energy balance. Let ε be the internal energy per unit mass, $\underline{\mathbf{q}}$ the heat flux vector, ϱ the current density. The energy balance equation reads then

$$\varrho\, \dot{\varepsilon} = \underset{\sim}{\boldsymbol{\sigma}} : (\underline{\mathbf{v}} \otimes \underline{\nabla}^c - \underset{\sim}{\boldsymbol{\upsilon}}) + \underset{\sim}{\boldsymbol{\mu}} : (\overset{\times}{\underline{\boldsymbol{\upsilon}}} \otimes \underline{\nabla}^c) - \operatorname{div}\, \underline{\mathbf{q}} \tag{2.21}$$

(any other inner heat supply is excluded for simplicity).

According to the thermodynamics of irreversible processes, the entropy principle is written

$$\varrho\, \dot{\eta} + \operatorname{div} \left(\frac{\underline{\mathbf{q}}}{T} \right) \geq 0, \tag{2.22}$$

where T denotes the temperature and η the entropy per unit mass.

Introducing the free energy $\psi = \varepsilon - \eta T$ and combining the energy and entropy equations, one derives the Clausius–Duhem inequality

$$-\varrho(\dot{\psi} + \eta T) + {}^{\sharp}\underset{\sim}{\boldsymbol{\sigma}} : ({}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{-1}) + {}^{\sharp}\underset{\sim}{\boldsymbol{\mu}} : ({}^{\sharp}\dot{\underset{\sim}{\boldsymbol{\Gamma}}}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{-1}) - \frac{1}{T}\, \underline{\mathbf{q}} \,.\, T\, \underline{\nabla}^c \geq 0, \tag{2.23}$$

where

$$\begin{aligned} {}^{\sharp}\underset{\sim}{\boldsymbol{\sigma}} &= \underset{\sim}{\mathbf{R}}^T\, \underset{\sim}{\boldsymbol{\sigma}}\, \underset{\sim}{\mathbf{R}}, \\ {}^{\sharp}\underset{\sim}{\boldsymbol{\mu}} &= \underset{\sim}{\mathbf{R}}^T\, \underset{\sim}{\boldsymbol{\mu}}\, \underset{\sim}{\mathbf{R}}, \end{aligned} \tag{2.24}$$

are rotated stress tensors with respect to the space frame $E^\sharp$ attached to the microstructure.

A material is said to be hyperelastic if its free energy and entropy are functions of ${}^\sharp\underset{\sim}{\mathbf{F}}$ and ${}^\sharp\underset{\sim}{\mathbf{\Gamma}}$ only. The Clausius–Duhem inequality (2.23) becomes

$$-\left(\varrho\frac{\partial\psi}{\partial\,{}^\sharp\underset{\sim}{\mathbf{F}}}-{}^\sharp\underset{\sim}{\boldsymbol{\sigma}}\,{}^\sharp\underset{\sim}{\mathbf{F}}^{-T}\right):{}^\sharp\dot{\underset{\sim}{\mathbf{F}}}-\left(\varrho\frac{\partial\psi}{\partial\,{}^\sharp\underset{\sim}{\mathbf{\Gamma}}}-{}^\sharp\underset{\sim}{\boldsymbol{\mu}}\,{}^\sharp\underset{\sim}{\mathbf{F}}^{-T}\right):{}^\sharp\dot{\underset{\sim}{\mathbf{\Gamma}}}$$
$$-\left(\varrho\,\eta+\varrho\frac{\partial\psi}{\partial T}\right)\dot{T}-\frac{1}{T}\underline{\mathbf{q}}.T\underline{\nabla}^c\geq 0.$$

Since this expression is linear in ${}^\sharp\dot{\underset{\sim}{\mathbf{F}}}$, ${}^\sharp\dot{\underset{\sim}{\mathbf{\Gamma}}}$ and $\dot{T}$, the last inequality implies

$$\eta=-\frac{\partial\psi}{\partial T} \tag{2.25}$$

and

$$\begin{aligned}{}^\sharp\underset{\sim}{\boldsymbol{\sigma}}&=\varrho\frac{\partial\psi}{\partial\,{}^\sharp\underset{\sim}{\mathbf{F}}}\,{}^\sharp\underset{\sim}{\mathbf{F}}^T,\\ {}^\sharp\underset{\sim}{\boldsymbol{\mu}}&=\varrho\frac{\partial\psi}{\partial\,{}^\sharp\underset{\sim}{\mathbf{\Gamma}}}\,{}^\sharp\underset{\sim}{\mathbf{F}}^T.\end{aligned} \tag{2.26}$$

2.3.2. Linear case; isotropic elasticity. Strain and torsion-curvature are small if $\|{}^\sharp\underset{\sim}{\mathbf{F}}-\underset{\sim}{\mathbf{1}}\|\ll 1$ and $\|{}^\sharp\underset{\sim}{\mathbf{\Gamma}}\|\,l\ll 1$, where l is a characteristic length. If, in addition, microrotations remain small, i.e. if $\|\underline{\mathbf{\Phi}}\|\ll 1$, then

$$\begin{aligned}\underset{\sim}{\mathbf{R}}&\simeq\underset{\sim}{\mathbf{1}}+\underline{\mathbf{1}}\times\underline{\mathbf{\Phi}}=\underset{\sim}{\mathbf{1}}-\underset{\sim}{\epsilon}\,\underline{\mathbf{\Phi}},\\ {}^\sharp\underset{\sim}{\mathbf{F}}&\simeq\underset{\sim}{\mathbf{1}}+\underline{\mathbf{u}}\otimes\underline{\nabla}+\underset{\sim}{\epsilon}\,\underline{\mathbf{\Phi}}=\underset{\sim}{\mathbf{1}}+\underset{\sim}{\mathbf{e}},\\ {}^\sharp\underset{\sim}{\mathbf{\Gamma}}&\simeq\underline{\mathbf{\Phi}}\otimes\underline{\nabla}=\underset{\sim}{\boldsymbol{\kappa}}.\end{aligned} \tag{2.27}$$

Furthermore, ${}^\sharp\underset{\sim}{\boldsymbol{\sigma}}\simeq\underset{\sim}{\boldsymbol{\sigma}}$ and ${}^\sharp\underset{\sim}{\boldsymbol{\mu}}\simeq\underset{\sim}{\boldsymbol{\mu}}$. Accordingly, for linear elasticity, two four-rank elasticity tensors are introduced

$$\begin{aligned}\underset{\sim}{\boldsymbol{\sigma}}&=\underset{\approx}{\mathbf{E}}:\underset{\sim}{\mathbf{e}},\\ \underset{\sim}{\boldsymbol{\mu}}&=\underset{\approx}{\mathbf{C}}:\underset{\sim}{\boldsymbol{\kappa}}\end{aligned} \tag{2.28}$$

(no coupling between strain and torsion-curvature is possible as soon as point symmetry is assumed, even for the less symmetric solid [18]). Some symmetry properties of these tensors are derived from the hyperelasticity conditions (2.26)

$$E_{ijkl}=E_{klij}\qquad\text{and}\qquad C_{ijkl}=C_{klij}\,. \tag{2.29}$$

Further symmetry conditions can be obtained if material symmetries are taken into account. The form of the Cosserat elasticity tensors for all symmetry classes

has been established by KESSEL [18]. In the case of isotropic elasticity, the two classical Lamé constants λ, μ are complemented by 4 additional parameters [12]

$$\begin{aligned} \underset{\sim}{\sigma} &= \lambda \underset{\sim}{1} \operatorname{Tr} \underset{\sim}{e} + 2\mu \{\underset{\sim}{e}\} + 2\mu_c \}\underset{\sim}{e}\{ , \\ \underset{\sim}{\mu} &= \alpha \underset{\sim}{1} \operatorname{Tr} \underset{\sim}{\kappa} + 2\beta \{\underset{\sim}{\kappa}\} + 2\gamma \}\underset{\sim}{\kappa}\{ . \end{aligned} \tag{2.30}$$

2.4. Elastoplastic Cosserat single crystals

The works of SAWCZUK [19], LIPPMANN [20] and BESDO [21] are the first milestones in the plasticity theory of Cosserat continua at small strains. In the case of single crystals we resort to recent results in the Cosserat theory at large strains [22].

2.4.1. Strain decomposition. In single crystals, non-homogeneous plastic deformations may induce non-homogeneous permanent lattice rotations, which are associated with plastic lattice curvature. That is why elastic and plastic Cosserat deformations and curvatures are introduced : ${}^{\sharp}\underset{\sim}{\mathbf{F}}^e$, ${}^{\sharp}\underset{\sim}{\mathbf{F}}^p$, ${}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^e$ and ${}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^p$. By means of *elastic* strains, free energy can be stored *without* intrinsic dissipation, i.e. without dissipation of power of deformation. The plastic strain rates can occur only together with the intrinsic dissipation rate. Strain partition rules must then be proposed. The most general decomposition of the strains ${}^{\sharp}\underset{\sim}{\mathbf{F}}$ and ${}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}$ reads:

$${}^{\sharp}\underset{\sim}{\mathbf{F}} = {}^{\sharp}\underset{\sim}{\hat{\mathbf{F}}}({}^{\sharp}\underset{\sim}{\mathbf{F}}^e,\ {}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^e,\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^p,\ {}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^p), \tag{2.31}$$

$${}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}} = {}^{\sharp}\underset{\sim}{\hat{\boldsymbol{\Gamma}}}({}^{\sharp}\underset{\sim}{\mathbf{F}}^e,\ {}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^e,\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^p,\ {}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^p). \tag{2.32}$$

The multiplicative decomposition proposed in [23] is adopted for the partially pure elastic materials under consideration, but only for the Cosserat deformation:

$${}^{\sharp}\underset{\sim}{\mathbf{F}} = {}^{\sharp}\underset{\sim}{\mathbf{F}}^e\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^p . \tag{2.33}$$

The expression

$${}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^{-1} = {}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}^{e}\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e-1} + {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e}\ {}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}^{p}\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^{p-1}\ {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e-1} \tag{2.34}$$

has to be substituted in the Clausius–Duhem inequality (2.23). This can be done also with the strain-functions (2.31) and (2.32) using the partial derivatives with respect to the elastic and plastic strain parts. At a dependence of the strain-functions ${}^{\sharp}\underset{\sim}{\hat{\mathbf{F}}}$ and ${}^{\sharp}\underset{\sim}{\hat{\boldsymbol{\Gamma}}}$ only on the corresponding elastic parts (besides the plastic ones), substitution into the fundamental restriction (2.23) gives the hyperelastic constitutive equations in a general form [22]:

$$\begin{aligned} {}^{\sharp}\underset{\sim}{\sigma} &= \varrho \frac{\partial \psi}{\partial\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^e} : \left(\frac{\partial\, {}^{\sharp}\underset{\sim}{\hat{\mathbf{F}}}}{\partial\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^e} \right)^{-1} {}^{\sharp}\underset{\sim}{\mathbf{F}}^T , \\ {}^{\sharp}\underset{\sim}{\mu} &= \varrho \frac{\partial \psi}{\partial\, {}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^e} : \left(\frac{\partial\, {}^{\sharp}\underset{\sim}{\hat{\boldsymbol{\Gamma}}}}{\partial\, {}^{\sharp}\underset{\sim}{\boldsymbol{\Gamma}}^e} \right)^{-1} {}^{\sharp}\underset{\sim}{\mathbf{F}}^T . \end{aligned} \tag{2.35}$$

Metals are materials which can behave in the current configuration purely elastically. Therefore the most natural assumption is that the elastic relations still have the form

$$
\begin{aligned}
{}^{\sharp}\underset{\sim}{\sigma} &= \varrho \frac{\partial \psi}{\partial\, {}^{\sharp}\underset{\sim}{F}^{e}}\, {}^{\sharp}\underset{\sim}{F}^{eT}, \\
{}^{\sharp}\underset{\sim}{\mu} &= \varrho \frac{\partial \psi}{\partial\, {}^{\sharp}\underset{\sim}{\Gamma}^{e}}\, {}^{\sharp}\underset{\sim}{F}^{eT},
\end{aligned}
\tag{2.36}
$$

as in the pure hyperelastic case, see (2.26). Then, setting the special constitutive relations (2.36) equal to the general hyperelastic forms (2.35), one obtains conditions for the strain-functions (2.31) and (2.32), from which the representation (2.33) and a decomposition of the entire wryness tensor can be derived [22]:

$$
{}^{\sharp}\underset{\sim}{\Gamma} = {}^{\sharp}\underset{\sim}{\Gamma}^{e}\, {}^{\sharp}\underset{\sim}{F}^{p} + {}^{\sharp}\underset{\sim}{\Gamma}^{p}. \tag{2.37}
$$

An elastic-plastic decomposition of the rotation $\underset{\sim}{R}$ [24], as of the displacement, is not recommendable, because these non-objective variables can not be connected with the quantities of energy and dissipation. Such a connection is possible only on the level of strains. The decomposition (2.37) has been assumed in [25]. Then the elastic constitutive equations (2.36) follow necessarily. The decompositions (2.33) and (2.37) enable one to define at each point the released state of the crystal for which stresses and couple stresses are removed and plastic deformation and curvature only remain. This is the reason why (2.37) is more suitable for crystals than a purely additional decomposition [26].

2.4.2. Kinematics of elastoplastic Cosserat single crystals. The plastic deformation of single crystals is the result of slip processes on slip systems. For each slip system s, we define

$$
\underline{m}^{s} = \underline{b}^{s} / \|\underline{b}^{s}\|, \tag{2.38}
$$

where $\underline{b}^{s}$ is the Burgers vector. $\underline{z}^{s}$ is the unit vector normal to the slip plane. As a result, the plastic strain rate takes the form

$$
{}^{\sharp}\dot{\underset{\sim}{F}}^{p}\, {}^{\sharp}\underset{\sim}{F}^{p-1} = \sum_{s \in S} \dot{\gamma}^{s}\, {}^{\sharp}\underset{\sim}{P}^{s}. \tag{2.39}
$$

γ^{s} is the amount of slip for the system s. ${}^{\sharp}\underset{\sim}{P}^{s}$ is given by the kinematics of slip

$$
{}^{\sharp}\underset{\sim}{P}^{s} = {}^{\sharp}\underline{m}^{s} \otimes {}^{\sharp}\underline{z}^{s}, \tag{2.40}
$$

where ${}^{\sharp}\underline{z}^{s} = \underset{\sim}{R}^{T}\, \underline{z}^{s}$. If we go back to the Eulerian representation

$$
\underline{v} \otimes \underline{\nabla}^{c} = \dot{\underset{\sim}{F}}\, \underset{\sim}{F}^{-1} = \dot{\underset{\sim}{R}}\, \underset{\sim}{R}^{T} + \underset{\sim}{R}\, {}^{\sharp}\dot{\underset{\sim}{F}}^{e}\, {}^{\sharp}\underset{\sim}{F}^{e-1}\, \underset{\sim}{R}^{T} + \underset{\sim}{R}\, {}^{\sharp}\underset{\sim}{F}^{e}\, {}^{\sharp}\dot{\underset{\sim}{F}}^{p}\, {}^{\sharp}\underset{\sim}{F}^{p-1}\, {}^{\sharp}\underset{\sim}{F}^{e-1}\, \underset{\sim}{R}^{T},
$$

we can split the last expression into its symmetric and skew-symmetric parts:

$$\{\underset{\sim}{\mathbf{v}} \otimes \nabla^c\} = \{\underset{\sim}{\mathbf{R}}\, {}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}^{e}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e-1}\, \underset{\sim}{\mathbf{R}}^{T}\} + \sum_{s\in S} \dot{\gamma}^s \{\, {}^{\star}\underline{\mathbf{m}}^s \otimes {}^{\star}\underline{\mathbf{z}}^s\} \tag{2.41}$$

and

$$\}\underline{\mathbf{v}} \otimes \underline{\nabla}^c\{ - \dot{\underset{\sim}{\mathbf{R}}}\, \underset{\sim}{\mathbf{R}}^{T} = \}\underset{\sim}{\mathbf{R}}\, {}^{\sharp}\dot{\underset{\sim}{\mathbf{F}}}^{e}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e-1}\, \underset{\sim}{\mathbf{R}}^{T}\{ + \sum_{s\in S} \dot{\gamma}^s \}\, {}^{\star}\underline{\mathbf{m}}^s \otimes {}^{\star}\underline{\mathbf{z}}^s\{\,, \tag{2.42}$$

where we have noted

$${}^{\star}\underline{\mathbf{m}}^s = \underset{\sim}{\mathbf{R}}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e}\, {}^{\sharp}\underline{\mathbf{m}}^s \qquad \text{and} \qquad {}^{\star}\underline{\mathbf{z}}^s = \underset{\sim}{\mathbf{R}}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e-T}\, {}^{\sharp}\underline{\mathbf{z}}^s\,. \tag{2.43}$$

Equation (2.42) clearly shows that the relative rotation rate of material lines with respect to the microstructure is due to the lattice rotation associated with slip processes, if elastic contributions are neglected.

We would like to compare the proposed formulation with Mandel's work. We are working with invariant tensors written in the microstructure space frame in order to get rid of undetermined rotations. An equivalent method is to deal with the so-called isoclinic configuration introduced by TEODOSIU [27] and MANDEL [23]. Their description reads

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{E}}\, \underset{\sim}{\mathbf{P}}\,, \tag{2.44}$$

where the rotation $\underset{\sim}{\mathbf{R}}^{\text{isoclinic}}$ appearing in the polar decomposition of $\underset{\sim}{\mathbf{E}}$ links the isoclinic reference frame to the working space frame. As a result, comparing (2.33) and (2.44) one can think of the equivalence

$$\underset{\sim}{\mathbf{E}} = \underset{\sim}{\mathbf{R}}\, {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e}\,. \tag{2.45}$$

However, considering the respective polar decompositions

$$\underset{\sim}{\mathbf{E}} = \underset{\sim}{\mathbf{R}}^{\text{isoclinic}}\, \underset{\sim}{\mathbf{U}}^{e} \qquad \text{and} \qquad {}^{\sharp}\underset{\sim}{\mathbf{F}}^{e} = \underset{\sim}{\mathbf{R}}^{e}\, \underset{\sim}{\mathbf{U}}^{e}$$

we should have then

$$\underset{\sim}{\mathbf{R}}^{\text{isoclinic}} = \underset{\sim}{\mathbf{R}}\, \underset{\sim}{\mathbf{R}}^{e}\,. \tag{2.46}$$

Regarding the elastic behaviour in the classical case, lattice vectors are material vectors with respect to the intermediate released configuration. Within the proposed framework this is not exactly true any more. There is an additional rotation $\underset{\sim}{\mathbf{R}}^{e}$ of material fibres with respect to the microstructure, that could be attributed to the presence of heterogeneities. Nevertheless the constitutive theory must be such that $\underset{\sim}{\mathbf{R}}^{e}$ remains a corrective term.

The plastic lattice curvature and torsion are due to the presence of dislocations with a non-vanishing resulting Burgers vector (see Sec. 3). The curvature planes and torsion axes are therefore related to crystallographic directions. They can be represented by the effect of continuous edge and screw dislocations for each slip system. That is why we propose the following kinematics for the plastic wryness

$$\sharp\dot{\underset{\sim}{\Gamma}}^p \, \sharp\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s\in S} \frac{\dot{\theta}^s}{l} \, \sharp\underset{\sim}{\mathbf{Q}}^s . \tag{2.47}$$

The θ^s are angles that measure the plastic curvature and torsion over a characteristic length l. Explicit forms for $\sharp\underset{\sim}{\mathbf{Q}}^s$ are given in Sec. 4.1.

2.5. Dissipation

In the Clausius–Duhem inequality (2.23), a contribution to the overall entropy production is due to the development of rotation gradients. If no hardening variables are introduced, the intrinsic dissipation rate is

$$\begin{aligned}\dot{D} = {} & \underset{\sim}{\boldsymbol{\sigma}} : \left(\underset{\sim}{\mathbf{R}} \, \sharp\underset{\sim}{\mathbf{F}}^e \, \sharp\dot{\underset{\sim}{\mathbf{F}}}^p \, \sharp\underset{\sim}{\mathbf{F}}^{p-1} \, \sharp\underset{\sim}{\mathbf{F}}^{e-1} \, \underset{\sim}{\mathbf{R}}^T\right) \\ & + \underset{\sim}{\boldsymbol{\mu}} : \left(\underset{\sim}{\mathbf{R}} \, \sharp\underset{\sim}{\Gamma}^e \, \sharp\dot{\underset{\sim}{\mathbf{F}}}^p \, \sharp\underset{\sim}{\mathbf{F}}^{p-1} \, \sharp\underset{\sim}{\mathbf{F}}^{e-1} \, \underset{\sim}{\mathbf{R}}^T\right) \\ & + \underset{\sim}{\boldsymbol{\mu}} : \left(\underset{\sim}{\mathbf{R}} \, \sharp\dot{\underset{\sim}{\Gamma}}^p \, \sharp\underset{\sim}{\mathbf{F}}^{-1} \, \underset{\sim}{\mathbf{R}}^T\right) .\end{aligned}$$

Taking (2.39) and (2.47) into account,

$$\begin{aligned}\dot{D} = {} & \sum_{s\in S} \dot{\gamma}^s \, \underset{\sim}{\boldsymbol{\sigma}} : {}^\star\underset{\sim}{\mathbf{P}}^s \\ & + \sum_{s\in S} \dot{\theta}^s \, \underset{\sim}{\boldsymbol{\mu}} : {}^\star\underset{\sim}{\mathbf{Q}}^s \\ & + \underset{\sim}{\boldsymbol{\mu}} : \left(\underset{\sim}{\mathbf{R}} \, \sharp\underset{\sim}{\Gamma}^e \, \sharp\dot{\underset{\sim}{\mathbf{F}}}^p \, \sharp\underset{\sim}{\mathbf{F}}^{p-1} \, \sharp\underset{\sim}{\mathbf{F}}^{e-1} \, \underset{\sim}{\mathbf{R}}^T\right),\end{aligned} \tag{2.48}$$

where

$$\begin{aligned}{}^\star\underset{\sim}{\mathbf{P}}^s &= \underset{\sim}{\mathbf{R}} \, \sharp\underset{\sim}{\mathbf{F}}^e \, \sharp\underset{\sim}{\mathbf{P}}^s \, \sharp\underset{\sim}{\mathbf{F}}^{e-1} \, \underset{\sim}{\mathbf{R}}^T , \\ {}^\star\underset{\sim}{\mathbf{Q}}^s &= \underset{\sim}{\mathbf{R}} \, \sharp\underset{\sim}{\mathbf{F}}^e \, \sharp\underset{\sim}{\mathbf{Q}}^s \, \sharp\underset{\sim}{\mathbf{F}}^{e-1} \, \underset{\sim}{\mathbf{R}}^T .\end{aligned} \tag{2.49}$$

Three terms appear in the dissipation. The first one is the classical one: slip processes due to irreversible dislocation motion are dissipative. The second one is due to the evolution of plastic curvature and torsion. It is clear that homogeneous lattice rotation is definitely not a dissipative process, but plastic curvature due to non-homogeneous lattice rotation is related to the existence of

accommodation dislocations and therefore must be associated with dissipation. This will be investigated in Sec. 4.4. The last term reveals the independence of the elastic curvature-torsion measure from plastic changes of the material lines in the intermediate configuration. This is due to the lattice concept, which means that the elastic behaviour, given in (2.36), is primarily not influenced by plastic straining. Thus, the elastic strain measures are related to lattice line-elements and their reference to material lines produce an additional term in the plastic wryness rate. However, at small elastic strains, this term vanishes.

3. Closure of the continuum theory of dislocations

3.1. Closure problem of the continuum theory of dislocations

The origin of the continuum theory of dislocations goes back to Nye's epoch-making work on *"Some geometrical relations in dislocated crystals"* [3]. He introduced the dislocation density tensor $\underset{\sim}{\alpha}$ which will be presented in Sec. 3.2 and he established a link between $\underset{\sim}{\alpha}$ and lattice curvature. KRÖNER [28] proposed a general presentation of the theory and gave the set of partial differential equations to be solved in the linear static case for a given distribution of dislocations, and here for an infinite body

$$
\begin{aligned}
\underset{\sim}{\beta} &= \underset{\sim}{\beta}^e + \underset{\sim}{\beta}^p, \\
\underset{\sim}{\sigma} &= \underset{\approx}{\mathbf{E}}\,\{\underset{\sim}{\beta}^e\}, \\
\underline{\mathrm{div}}\,\underset{\sim}{\sigma} &= 0, \\
\underset{\sim}{\mathrm{curl}}\,\underset{\sim}{\beta}^e &= \underset{\sim}{\alpha},
\end{aligned}
\tag{3.1}
$$

where $\underset{\sim}{\beta} = \underline{\mathbf{u}} \otimes \underline{\nabla} = u_{i,j}\ \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j$. In this part, we use Kröner's notations for historical reasons. It must be noted that, strictly speaking, the non-objective quantity $\underset{\sim}{\beta}$ cannot be decomposed entirely into an elastic and plastic part but the usual notations of the continuum theory of dislocations and of classical plasticity theory can be reconciled by the concept of isoclinic configuration as it was done in [29]. The continuum theory of dislocations is a way to think of dislocation theory as of a physical field theory. The system (3.1) enables us to find the stress-strain field around dislocations for some given arrangements. However such a theory cannot bridge the gap between the dislocation theory and plasticity theory since it does not predict the motion of dislocations. The dislocation distribution must be known at each step. In the dynamic theory of continuous distributions of dislocations, KRÖNER [28] and MURA [30, 31] introduce the dislocation flux tensor $\underset{\approx}{\mathbf{V}}$ which is related to the plastic deformation rate $\dot{\underset{\sim}{\beta}}^p$ by

$$
\dot{\underset{\sim}{\beta}}^p = -\left(\underset{\approx}{\epsilon} : \underset{\approx}{\mathbf{V}}\right)^T \tag{3.2}
$$

and we still have

$$\dot{\underset{\sim}{\alpha}} = -\operatorname{curl}\dot{\underset{\sim}{\beta}}^{p}. \tag{3.3}$$

For a single dislocation, the dislocation flux tensor reads

$$\underset{\approx}{\mathbf{V}} = \underline{\mathbf{v}} \otimes \underline{\xi} \otimes \underline{\mathbf{b}}, \tag{3.4}$$

$\underline{\mathbf{v}}$ is the dislocation velocity vector, $\underline{\xi}$ is the dislocation line vector and $\underline{\mathbf{b}}$ the Burgers vector. In this case stress and strain can be obtained provided that $\underset{\sim}{\alpha}$ and $\underset{\approx}{\mathbf{V}}$ are given at each time, which is of no help to derive a plasticity theory. For, the continuum theory of dislocations, even in more recent review articles like [33], does not provide constitutive equations. As pointed out by HAHN and JAUNZEMIS [34], in a complete theory of dislocations, the density and motion of dislocations should be derivable from the knowledge of initial conditions (and boundary conditions) only. This is what we call the closure problem of the continuum theory of dislocations.

Two attempts to derive the missing constitutive equations must be mentioned. On the one hand MURA [35] showed how the von Mises yield criterion and Prandtl–Reuss relations can be explained in terms of the dislocation velocity tensor and a so-called "gliding force". The underlying constitutive assumption is a linear relation between $\underset{\approx}{\mathbf{V}}$ and the gliding force. According to [36] and [37], constitutive equations are also necessary to link plasticity and dislocation theories. On the other hand, HAHN and JAUNZEMIS [34] distinguish mobile dislocations (M) from immobile ones (I) with common line and Burgers vectors. $A^{ab} = A_I^{ab} + A_M^{ab}$ is the number of dislocations of Burgers vector $\underline{\mathbf{b}}^a$ and line vector $\underline{\xi}^b$. Using a large strain formulation, (3.1) combined with (3.4) yields

$$\dot{\underset{\sim}{\mathbf{F}}}^{p}\,\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{a,b} \underline{\mathbf{b}}^a \otimes (\underline{\xi}^b \times \underline{\mathbf{v}}^{ab}) A_M^{ab} = \sum_a A^a V^a\, \underline{\mathbf{b}}^a \otimes \underline{\mathbf{z}}^a, \tag{3.5}$$

where

$$A^a V^a\, \underline{\mathbf{z}}^a = \sum_b A_M^{ab}\, \underline{\xi}^b \times \underline{\mathbf{v}}^{ab}$$

is normal to the slip plane. Evolution equations are proposed for A_I^a and A_M^a. Isotropic and kinematic hardening and a viscous stress are also introduced in the modelling. Climb mechanisms are not considered.

3.2. Statistical description of dislocation distribution

The dislocation network and dislocation sources distribution within a considered single crystal volume element often is or becomes so intricate that an exact description of all dislocation lines and Burgers vectors must be abandoned. Instead some overall and statistical information about the distribution may be

sufficient for the modelling of the plastic behaviour of the element. The only known attempts to develop a complete statistical theory of dislocations go back to ZORSKI [38] and KRÖNER [39]. The systematic approach comes up against tremendous difficulties which are still not overcome. This explains why the concepts reviewed in this section are only rudimentary tools which do not exhaust the complexity of dislocation structures.

3.2.1. Dislocation density tensor and the continuum theory of dislocations. Within the framework of the continuum theory of dislocations, the characteristic size l of the volume element is taken large enough for the effects of the dislocations within it to be averaged. The distribution of dislocations is made continuous by letting $b = \|\underline{\mathbf{b}}\|$ approach zero and increasing the number n of dislocations of each kind so as to keep nb constant [3]. The definition of the Burgers vector can be extended to continuous distributions of dislocations [27]. For that purpose one refers to the kinematic description proposed by MANDEL [23] making use of the isoclinic configuration and of the strain partition given by (2.44). In (2.44), $\underset{\sim}{\mathbf{E}}$ relates the infinitesimal vectors $d\underline{\zeta}$ and $d\underline{\mathbf{x}}$, where $d\underline{\zeta}$ results from the cutting and releasing operations of the infinitesimal current lattice vector $d\underline{\mathbf{x}}$

$$d\underline{\zeta} = \underset{\sim}{\mathbf{E}}^{-1}\, d\underline{\mathbf{x}}\,. \tag{3.6}$$

It can be seen that the decomposition (2.44) actually goes back to [40].

Accordingly, if S is a smooth surface containing $\underline{\mathbf{x}}$ in the current configuration and bounded by the closed line c, the true Burgers vector is defined as in [27]

$$\underline{\mathbf{b}} = \oint_c \underset{\sim}{\mathbf{E}}^{-1}\, d\underline{\mathbf{x}}\,. \tag{3.7}$$

The application of Stokes' formula (A.19) leads to the definition of the so-called true dislocation density tensor

$$\underset{\sim}{\boldsymbol{\alpha}} = -\mathrm{curl}^{\mathrm{c}}\, \underset{\sim}{\mathbf{E}}^{-1} = \underset{\sim}{\mathbf{E}}^{-1} \times \underline{\nabla}^{c} = -\epsilon_{jkl}\, E^{-1}_{ik,l}\, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \tag{3.8}$$

such that

$$\underline{\mathbf{b}} = \int_S \underset{\sim}{\boldsymbol{\alpha}}\, \underline{\mathbf{n}}\, dS\,. \tag{3.9}$$

If the surface is infinitesimal of normal $\underline{\mathbf{n}}$, $d\underline{\mathbf{b}} = \underset{\sim}{\boldsymbol{\alpha}}\, \underline{\mathbf{n}}\, dS$ is the resulting true Burgers vector of dislocations crossing the surface dS. It is convenient to associate each component α_{ij} of the dislocation density tensor with a (super) dislocation characterized by its line vector $\underline{\mathbf{e}}_j$ and its Burgers vector $b_i\, \underline{\mathbf{e}}_i$ (no summation). As a result, the diagonal components of $\underset{\sim}{\boldsymbol{\alpha}}$ represent screw dislocations and the out-of-diagonal ones edge dislocations. For n dislocations per unit surface of Burgers vector $\underline{\mathbf{b}}$ and line vector $\underline{\xi}$, we have

$$\underset{\sim}{\boldsymbol{\alpha}} = n\, \underline{\mathbf{b}} \otimes \underline{\xi}\,. \tag{3.10}$$

3.2.2. Scalar dislocation densities and crystal plasticity. In the classical continuum theory of dislocations, the description of the dislocation distribution is restricted to the dislocation density tensor. It enables one to compute stress-strain fields for special distributions and even discrete dislocations for which $\underset{\sim}{\alpha}$ becomes the sum of Dirac's functions [28]. However the classical continuum theory of dislocations has failed to describe the elastoplastic behaviour of single crystals. The main reason is that the dislocation density tensor is not the relevant variable to explain the hardening processes. In [34], the kinematics of plastic deformation are derived from the dislocation velocity tensor and correspond exactly to the purely mechanical description of slip processes proposed by MANDEL [23]. The next step is the introduction of hardening variables as in the classical macroscopic plasticity theory. They are related to usual scalar dislocation densities that are commonly used by metal phycisists and which represent the total length of dislocation lines within a volume element. The multiplication and interaction of dislocations are responsible for the hardening of single crystals and the scalar densities are reliable measures for it. This type of description culminates with the work of MANDEL [23], ZARKA [41] and TEODOSIU and SIDOROFF [42]. In these theories the dislocation density tensor is not even mentioned since it is not the relevant quantity any more. Constitutive equations for hardening variables are proposed in a more or less phenomenological way and several elementary dislocation interaction processes are taken into account.

The main successes of these theories are the modelling of the tensile behaviour of single crystals, the lattice rotations [43] and the cyclic behaviour of single and polycrystals [44].

3.2.3. Proposed description. In this work we claim that both types of descriptions are required for the modelling of non-homogeneous deformation of single crystals. That is why the statistical description of dislocation distribution must contain at least:

- the dislocation density tensor $\underset{\sim}{\alpha}$ which accounts for the resulting Burgers vector across any infinitesimal surface,

and

- scalar dislocation densities ϱ^s or the associated hardening variables, for instance r^s and x^s already used in [45]. The kinematic hardening variables x^s are a measure for microscopically non-homogeneous spatial dislocation distributions that give rise to a vanishing resulting Burgers vector (dislocation cells...). Additional variables (densities of mobile and immobile dislocations...) may also be necessary.

It must be noted that the dislocation density tensor and the scalar dislocation densities are related, respectively, to the one-point and two-point dislocation correlations introduced by KRÖNER [39].

The scalar dislocation densities are necessary to account for the hardening or softening behaviour of the material whereas the dislocation density tensor may play a significant role when strong lattice incompatibilities are present.

3.3. Link between the dislocation density tensor and the lattice torsion-curvature tensor

3.3.1. Classical analysis at small strains and small rotations. NYE [3] introduces the rotation vector $\underline{\Phi}$ of the lattice and the curvature tensor $\underset{\sim}{\kappa} = \underline{\Phi} \otimes \underline{\nabla}$. At small strains and small rotations, the strain and rotation rate decomposition into elastic and plastic parts reads

$$\begin{aligned} \dot{\underset{\sim}{\beta}} &= \dot{\underset{\sim}{\beta}}^{e} + \dot{\underset{\sim}{\beta}}^{p} \\ &= \dot{\underset{\sim}{\varepsilon}} + \underset{\sim}{\omega} \\ &= \dot{\underset{\sim}{\varepsilon}}^{e} + \underset{\sim}{\omega}^{e} + \dot{\underset{\sim}{\varepsilon}}^{p} + \underset{\sim}{\omega}^{p} . \end{aligned} \tag{3.11}$$

$\underset{\sim}{\omega}^{p} = \underset{\sim}{\omega} - \underset{\sim}{\omega}^{e} = \underset{\sim}{\omega} - \underset{\sim}{1} \times \dot{\underline{\Phi}}$ represents the relative rotation of material lines with respect to the lattice. As a result, relation (3.8) becomes

$$\dot{\underset{\sim}{\alpha}} = \operatorname{curl} \dot{\underset{\sim}{\beta}}^{e} = \operatorname{curl} \dot{\underset{\sim}{\varepsilon}}^{e} + \operatorname{curl} \underset{\sim}{\omega}^{e} . \tag{3.12}$$

In a way similar to KRÖNER [28], we derive

$$\begin{aligned} \operatorname{curl} \underset{\sim}{\omega}^{e} &= \epsilon_{jkl}\, \omega_{ik,l}\, \underline{e}_i \otimes \underline{e}_j \\ &= -\epsilon_{jkl}\, \epsilon_{ikm}\, \dot{\Phi}_{m,l}\, \underline{e}_i \otimes \underline{e}_j \\ &= -\epsilon_{klj}\, \epsilon_{kmi}\, \dot{\kappa}_{ml}\, \underline{e}_i \otimes \underline{e}_j \\ &= -(\delta_{ml}\, \delta_{ij} - \delta_{il}\, \delta_{mj})\, \dot{\kappa}_{ml}\, \underline{e}_i \otimes \underline{e}_j \\ &= \dot{\underset{\sim}{\kappa}}^{T} - (\operatorname{Tr} \dot{\underset{\sim}{\kappa}})\, \underset{\sim}{1} . \end{aligned} \tag{3.13}$$

Neglecting the elastic strain, one obtains the expression proposed by NYE [3]

$$\underset{\sim}{\alpha} = \underset{\sim}{\kappa}^{T} - (\operatorname{Tr} \underset{\sim}{\kappa})\, \underset{\sim}{1} \tag{3.14}$$

and its reverse form

$$\underset{\sim}{\kappa} = \underset{\sim}{\alpha}^{T} - \frac{1}{2} (\operatorname{Tr} \underset{\sim}{\alpha})\, \underset{\sim}{1} . \tag{3.15}$$

Keeping the elastic term

$$\underset{\sim}{\alpha} = \operatorname{curl} \underset{\sim}{\varepsilon}^{e} + \underset{\sim}{\kappa}^{T} - (\operatorname{Tr} \underset{\sim}{\kappa})\, \underset{\sim}{1} . \tag{3.16}$$

3.3.2. Analysis for the Cosserat theory. Within the framework of the Cosserat theory for single crystals presented in Part 2, we propose the following definition for the true dislocation density tensor

$$\underset{\sim}{\alpha} = -\operatorname{curl}^{c} ({}^{\sharp}\underset{\sim}{\mathbf{F}}^{e-1}\, \underset{\sim}{\mathbf{R}}^{T}) . \tag{3.17}$$

We try now to link the dislocation density tensor and the wryness tensor. Equation (3.17) becomes

$$\underset{\sim}{\boldsymbol{\alpha}} = -\left(\epsilon_{jkl}\,\frac{\partial\, {}^{\natural}F^{e-1}_{im}}{\partial x_l}\,R_{km} + {}^{\natural}F^{e-1}_{im}\,\epsilon_{jkl}\,R^T_{mk,L}\,F^{-1}_{Ll}\right)\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \tag{3.18}$$

(the comma denotes again a derivative with respect to the reference configuration). Note that,

$$\underset{\sim}{\boldsymbol{\Gamma}} = \frac{1}{2}\underset{\approx}{\epsilon} : (\underset{\sim}{\mathbf{R}}\,(\underset{\sim}{\mathbf{R}}^T \otimes \underline{\nabla})) \implies \underset{\sim}{\mathbf{R}}\,(\underset{\sim}{\mathbf{R}}^T \otimes \underline{\nabla}) = \underset{\approx}{\epsilon}\,\underset{\sim}{\boldsymbol{\Gamma}} \tag{3.19}$$

or, in components,

$$R^T_{mk,l} = -R^T_{mu}\,\epsilon_{ukv}\,\Gamma_{vl}\,.$$

As a result, (3.17) can now be written

$$\begin{aligned}\underset{\sim}{\boldsymbol{\alpha}} &= \underset{\sim}{\mathbf{A}}^{el} - {}^{\natural}F^{e-1}_{im}\,R^T_{mu}\,\epsilon_{klj}\,\epsilon_{kvu}\,\Gamma_{vL}\,F^{-1}_{Ll}\,\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \\ &= \underset{\sim}{\mathbf{A}}^{el} + {}^{\natural}\underset{\sim}{\mathbf{F}}^{e-1}\,\underset{\sim}{\mathbf{R}}^T\left((\underset{\sim}{\boldsymbol{\Gamma}}\,\underset{\sim}{\mathbf{F}}^{-1})^T - \mathrm{Tr}\,(\underset{\sim}{\boldsymbol{\Gamma}}\,\underset{\sim}{\mathbf{F}}^{-1})\underline{\mathbf{1}}\right) \\ &= \underset{\sim}{\mathbf{A}}^{el} + {}^{\natural}\underset{\sim}{\mathbf{F}}^{e-1}\left(({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{-1})^T - \mathrm{Tr}\,({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{-1})\underline{\mathbf{1}}\right)\underset{\sim}{\mathbf{R}}^T,\end{aligned} \tag{3.20}$$

where $\underset{\sim}{\mathbf{A}}^{el} = \epsilon_{jkl}\dfrac{\partial\, {}^{\natural}F^{e-1}_{im}}{\partial x_l}\,R_{km}\,\underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j$. It can be checked that equation (3.16) is retrieved for small strains and rotations. We define

$${}^{\natural}\underset{\sim}{\boldsymbol{\alpha}} = \underset{\sim}{\boldsymbol{\alpha}}\,\underset{\sim}{\mathbf{R}} \tag{3.21}$$

and $\underset{\sim}{\mathbf{R}}\,{}^{\natural}\underset{\sim}{\mathbf{F}}^e\,\underset{\sim}{\boldsymbol{\alpha}}$ can be interpreted as the Cosserat counterpart of the local dislocation density tensor introduced in the classical continuum theory of dislocations.

Using the decomposition of the total wryness given by (2.37), the expression of the dislocation density tensor (3.20) becomes:

$$\begin{aligned}\underset{\sim}{\boldsymbol{\alpha}} = \underset{\sim}{\mathbf{A}}^{el} &+ {}^{\natural}\underset{\sim}{\mathbf{F}}^{e-1}\left(({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}^e\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{e-1})^T - \mathrm{Tr}\,({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}^e\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{e-1})\underline{\mathbf{1}}\right)\underset{\sim}{\mathbf{R}}^T \\ &+ {}^{\natural}\underset{\sim}{\mathbf{F}}^{e-1}\left(({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}^p\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{-1})^T - \mathrm{Tr}\,({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}^p\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{-1})\underline{\mathbf{1}}\right)\underset{\sim}{\mathbf{R}}^T.\end{aligned} \tag{3.22}$$

Considering now the released state for which force and couple stresses are removed, as defined at the end of Sec. 2.4.1., the remaining plastic curvature is related to the dislocation density tensor in the released state by:

$${}^{\natural}\hat{\underset{\sim}{\boldsymbol{\alpha}}} = ({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}^p\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{p-1})^T - \mathrm{Tr}\,({}^{\natural}\underset{\sim}{\boldsymbol{\Gamma}}^p\,{}^{\natural}\underset{\sim}{\mathbf{F}}^{p-1})\underline{\mathbf{1}}\,. \tag{3.23}$$

In particular, $\hat{\underset{\sim}{\boldsymbol{\alpha}}}$ is known for a given distribution of edge and screw dislocations. This result motivates the definition of the kinematics of plastic curvature evolution in Sec. 4.1. Note that, starting from the same definition (3.17), DŁUŻEWSKI [46] considers elastic and plastic dislocation tensors which are related to the contributions of elastic and plastic curvatures in equation (3.22).

3.4. Constrained Cosserat theories

The work of the Cosserat brothers was almost forgotten until GÜNTHER rediscovered it in 1958 [47]. Furthermore Günther has revealed the close link between the Cosserat theory and the continuum theory of dislocations which has been thriving since the early fifties.

This explains why the continuum theory of dislocations has often been further developed within the framework of a Cosserat continuum, for instance in [48]. In [8] discrete screw and edge dislocations are embedded in the Cosserat continuum. However the physical meaning of the directors remains unclear in these works: are they independent lattice vectors or material vectors? How do they rotate? In many cases the resulting framework is that of a constrained Cosserat theory like in [19]. The rotation rate of the directors is then given by the skew-symmetric part of the overall deformation gradient

$$\dot{\underline{\Phi}} = -\frac{1}{2}\underline{\underline{\epsilon}}\,(\dot{\underline{u}} \otimes \underline{\nabla}). \tag{3.24}$$

The curvature tensor that we denote $\underset{\sim}{\chi}$ in the constrained case then becomes

$$\dot{\underset{\sim}{\chi}} = \dot{\underline{\Phi}} \otimes \underline{\nabla} = -\frac{1}{2}\,\epsilon_{imn}\,u_{m,nj}\,\underline{e}_i \otimes \underline{e}_j\,. \tag{3.25}$$

It is clear that because of this constraint the directors generally are not lattice vectors. Besides the microrotations are entirely determined by the displacement field, which is not the case in the theory presented in Sec. 1. Considering the decomposition of the deformation and bend-twist tensors into elastic and plastic parts, MURA [35] and many authors consider

$$\dot{\underset{\sim}{\beta}} = \dot{\underset{\sim}{\beta}}^{e} + \dot{\underset{\sim}{\beta}}^{p} \qquad \text{and} \qquad \dot{\underset{\sim}{\chi}} = \dot{\underset{\sim}{\chi}}^{e} + \dot{\underset{\sim}{\chi}}^{p} \tag{3.26}$$

with

$$\dot{\underset{\sim}{\chi}}^{e} = \dot{\underline{\Phi}}^{e} = -\frac{1}{2}\underline{\underline{\epsilon}}\,\dot{\underset{\sim}{\beta}}^{e} \qquad \text{and} \qquad \dot{\underset{\sim}{\chi}}^{p} = \dot{\underline{\Phi}}^{p} = -\frac{1}{2}\underline{\underline{\epsilon}}\,\dot{\underset{\sim}{\beta}}^{p}\,, \tag{3.27}$$

so that

$$\dot{\underline{\Phi}}^{e} \otimes \underline{\nabla} + \dot{\underline{\Phi}}^{p} \otimes \underline{\nabla} = \dot{\underset{\sim}{\chi}}\,, \tag{3.28}$$

which also implies the constraint (3.24). As for them, KOSSECKA and DE WIT [33] define

$$\begin{aligned} \underset{\sim}{\alpha}^{T} &= \epsilon_{pkm}\left(\beta^{p}_{lk,m} + \epsilon_{klq}\,\chi^{p}_{qm}\right)\underline{e}_p \otimes \underline{e}_l \\ &= \underset{\sim}{\mathrm{curl}}\,\{\underset{\sim}{\beta}^{p}\} + \underset{\sim}{\chi}^{pT} - \mathrm{Tr}\,\underset{\sim}{\chi}^{p}\,\underset{\sim}{1}\,. \end{aligned} \tag{3.29}$$

Finally they interpret $(\underset{\sim}{\mathrm{curl}}\{\underset{\sim}{\chi}^p\})^T$ as the disclination density tensor. However, these formula are not derived from a precise definition of the Burgers vector like in (3.7) or (3.17) and are therefore difficult to assess.

The main advantage of the previous restricted Cosserat theories is that no constitutive equations are required for the plastic curvature. But it must be noted that the expression of the dislocation density tensor (3.16) or (3.20) involves the total torsion-curvature tensor. As a result, nothing is known *a priori* about the elastic and plastic relative contributions, so that constitutive equations with a yield criterion for the plastic curvature may be necessary.

However, looking at Eq. (3.22) may lead one to propose the following relation:

$$(\sharp\underset{\sim}{\boldsymbol{\Gamma}}^e\ \sharp\underset{\sim}{\mathbf{F}}^{e-1})^T - \mathrm{Tr}\,(\sharp\underset{\sim}{\boldsymbol{\Gamma}}^e\ \sharp\underset{\sim}{\mathbf{F}}^{e-1})\,\underset{\sim}{\mathbf{1}} = -\sharp\underset{\sim}{\mathbf{F}}^e\,\underset{\sim}{\mathbf{A}}^{el}\,\underset{\sim}{\mathbf{R}}, \tag{3.30}$$

which can be regarded as a definition for $\underset{\sim}{\boldsymbol{\Gamma}}^e$. If we still accept the decomposition (2.37), $\underset{\sim}{\boldsymbol{\Gamma}}^p$ can be deduced. In this case, there is no need for additional constitutive equations to close the problem. Nevertheless, it is not sure that Eq. (2.36) can be derived from this definition of the elastic wryness and, consequently, (2.37) does not necessarily hold. As a result, this definition is abandoned and Eq. (3.30) will not be used in the following. Instead we will stick to relations (2.33), (2.37), (2.39) and (2.47), and propose constitutive equations in Sec. 4. These constitutive equations will allow us to take the influence of plastic curvature on the hardening of the material into account.

3.5. Geometrically necessary dislocations and statistically stored dislocations

According to ASHBY [49], dislocations become stored in a plastically non-homogeneous solid for two reasons: dislocations are either required for the compatible deformation of various parts of the specimen or they accumulate by trapping each other in a random way. This gives rise on the one hand to the density ϱ_G of so-called geometrically necessary dislocations and on the other hand, to the density ϱ_S of statistically stored dislocations. The density ϱ_G can be computed approximately in some situations like plastic bending or punching. This variable comes directly from the continuum theory of dislocations and corresponds to the components of the dislocation density tensor $\underset{\sim}{\boldsymbol{\alpha}}$. In Sec. 4 we will introduce additional inner variables which are directly related to the density ϱ_G of geometrically necessary dislocations for each slip system.

In contrast, the density ϱ_S belongs to the second group of variables that have been listed in Sec. 3.2, namely the hardening variables. However, as shown by Ashby in the case of two-phase alloys, geometrically necessary dislocations may lead to additional hardening. In Sec. 4 we will try to model this coupling effect between the two types of variables that describe the dislocation distribution.

The relative importance of ϱ_G and ϱ_S depends on the amount of overall plastic deformation, and on the type of solicitation. Clearly ϱ_G can dominate in the case of strong deformation gradients.

These considerations have led FLECK, MÜLLER, ASHBY and HUTCHINSON [50] to apply a so-called strain-gradient plasticity theory to the tension and torsion of copper wires with various diameters. The model is equivalent to a constrained Cosserat theory first proposed in [19]. The J_2-theory is extended to couple stresses in a way similar to [51]. However the modelling becomes questionable when applied to wires with diameters comparable to the grain size. In that case the constrained rotations of the model have nothing to do with local lattice rotations, as explained in Sec. 3.4, and the associated curvature is not a relevant variable.

4. Explicit constitutive equations

We propose a set of constitutive equations for the elastoviscoplastic deformation and intrinsic curvature of metal single crystals.

4.1. Kinematics of plastic deformation and curvature

The plastic flow due to slip on various slip systems has been studied in Sec. 2.4.2 (Eq. (2.39)). Similarly, an expression of the plastic curvature evolution has been proposed (Eq. (2.47)). An expression of ${}^\sharp\underset{\sim}{\mathbf{Q}}^s$ is now derived from the analysis of the dislocation density tensor in Sec. 3.3.2. The scalar γ^s represents the amount of slip due to the passage of dislocations of type s through the volume element, as for them the scalars θ^s represent the plastic curvature due to dislocations trapped in the volume element of characteristic length l. When stresses and couple stresses are released, the elastic contributions in Eq. (3.22) disappear so that a direct relation between residual plastic curvature and the dislocation density tensor is obtained (Eq. (3.23)). We consider then that $\underset{\sim}{\boldsymbol{\alpha}}$ can be decomposed into the contributions of edge and screw dislocations and we give in the following the curvature and torsion axes in the two cases. The amounts of curvature θ^s will be computed using constitutive equations proposed in the next section.

Curvature due to edge dislocations ($\perp$)

For edge dislocations, ${}^\sharp\underset{\sim}{\boldsymbol{\alpha}} = b\,{}^\sharp\underline{\mathbf{m}} \otimes {}^\sharp\underline{\xi}$.

$\underline{\xi}$ is the dislocation line vector and the normal to the glide plane is defined as

$$\underline{\mathbf{z}} = \underline{\mathbf{m}} \times \underline{\xi}. \tag{4.1}$$

The associated curvature is shown in Fig. 1, so that we take

$${}^\sharp\underset{\sim}{\mathbf{Q}}_\perp = {}^\sharp\underline{\xi} \otimes {}^\sharp\underline{\mathbf{m}}. \tag{4.2}$$

Arrays of edge dislocations of the same type give rise to lattice curvature in the plane $(\underline{\mathbf{m}}, \underline{\mathbf{b}})$. The rotation vector $\underline{\boldsymbol{\Phi}}$ has the same direction as the dislocation line vector.

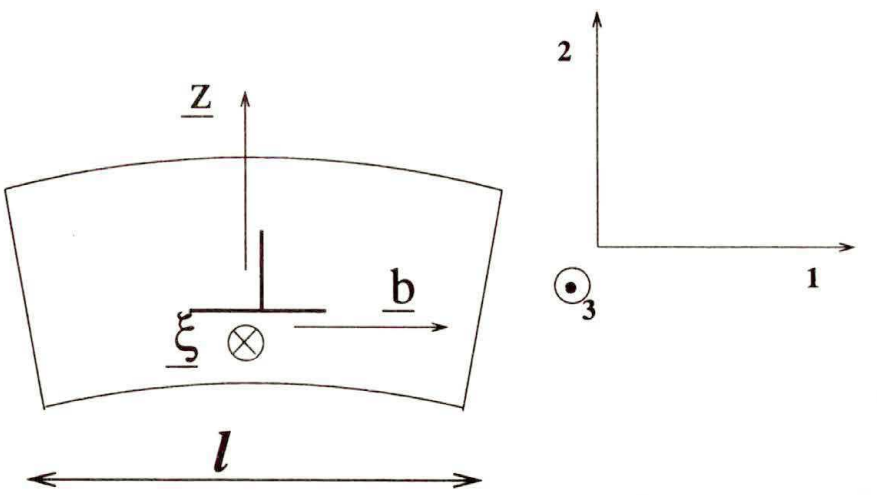

FIG. 1. Curvature due to edge dislocations.

Torsion due to screw dislocations ($\odot$)

For a screw dislocation, ${}^\sharp\underset{\sim}{\boldsymbol{\alpha}} = b\,{}^\sharp\underline{\mathbf{m}} \otimes {}^\sharp\underline{\mathbf{m}}$.

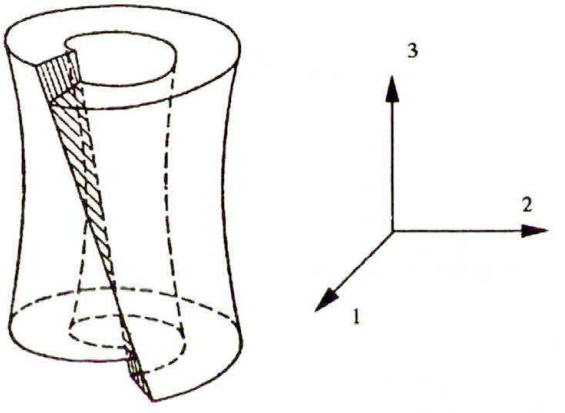

FIG. 2. Curvature due to a screw dislocations, after releasing the end couples (from [53]).

The associated curvature can be seen in Fig. 2, so that we take

$$ {}^\sharp\underset{\sim}{\mathbf{Q}}_\odot = \frac{1}{2}\underset{\sim}{\mathbf{1}} - {}^\sharp\underline{\mathbf{m}} \otimes {}^\sharp\underline{\mathbf{m}}. \tag{4.3} $$

The sign conventions for ${}^\sharp\underset{\sim}{\mathbf{Q}}_\perp$ and ${}^\sharp\underset{\sim}{\mathbf{Q}}_\odot$ are such that $\theta_\perp$ and $\theta_\odot$ are positive in Figs. 1 and 2. As a result, screw dislocations cause lattice torsion about the three reference axes. KRÖNER [28] noticed that a planar array of crossed screw dislocations with perpendicular Burgers vectors produces a twist of the lattice

about the third direction. This is equivalent to a grain boundary of the second kind. Grain boundaries of the first kind are generated by an array of edge dislocations with parallel Burgers and line vectors. Note that the result (4.3) is different from that proposed in [52], which gives no torsion with respect to the dislocation line axis. This seems to hold only when the couple that can be derived from the classical stress field around a screw dislocation is not released [53, 32]. Our expression (3.22) is derived from an extension of the definition of the Burgers vector for continuously distributed dislocations.

Lastly, we give the proposed kinematics of the plastic lattice torsion-curvature

$$(4.4) \qquad {}^{\natural}\dot{\underset{\sim}{\Gamma}}^{p}\ {}^{\natural}\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s\in S}\left(\frac{\dot{\theta}^s_{\perp}}{l}\ {}^{\natural}\underline{\xi}^s \otimes {}^{\natural}\underline{\mathbf{m}}^s + \frac{\dot{\theta}^s_{\odot}}{l}\left(\frac{1}{2}\underset{\sim}{\mathbf{1}} - {}^{\natural}\underline{\mathbf{m}}^s \otimes {}^{\natural}\underline{\mathbf{m}}^s\right)\right).$$

4.2. Generalized Schmid's law

4.2.1. Peach and Koehler's force. KRÖNER [54] shows that Peach and Koehler's formula giving the force on a dislocation $(\underline{\mathbf{b}}, \underline{\boldsymbol{\xi}})$ due to a stress field $\underset{\sim}{\boldsymbol{\sigma}}$ applies also for a non-symmetric stress tensor. But it is important to derive again the formula taking care of any transposition. The force $\underline{\mathbf{f}}$ per unit length of dislocation is defined, for a unit length of dislocation, through

$$(4.5) \qquad \underline{\mathbf{f}} \,.\, d\underline{\mathbf{x}} = \underline{\mathbf{b}} \,.\, (\underset{\sim}{\boldsymbol{\sigma}}\,\underline{\mathbf{n}})\, dS = ((\underline{\mathbf{b}}\,\underset{\sim}{\boldsymbol{\sigma}}) \times \underline{\boldsymbol{\xi}}) \,.\, d\underline{\mathbf{x}},$$

where

$$(4.6) \qquad \underline{\mathbf{n}}\, dS = \underline{\boldsymbol{\xi}} \times d\underline{\mathbf{x}}.$$

The dislocation can move in its plane only if the component of the force in the glide plane

$$(4.7) \qquad b\tau = \underline{\mathbf{f}} \,.\, (\underline{\mathbf{n}} \times \underline{\boldsymbol{\xi}}) = \underset{\sim}{\boldsymbol{\sigma}} : (\underline{\mathbf{b}} \otimes \underline{\mathbf{n}})$$

reaches a threshold. This is the physical meaning of Schmid's criterion. We will use this criterion to compute the slip rate on slip system s

$$(4.8) \qquad \dot{\gamma}^s = \left(\frac{\mathrm{Max}\,(0,\ |\tau^s - x^s| - r^s)}{k^s}\right)^{n^s} \mathrm{sign}\,(\tau^s - x^s),$$

where $\tau^s = {}^{\natural}\underset{\sim}{\boldsymbol{\sigma}} : {}^{\natural}\underset{\sim}{\mathbf{P}}^s$ according to (4.7), and x^s and r^s are internal kinematic and isotropic hardening variables. x^s and r^s represent, respectively, the back-stress and the yield threshold, which are supposed to describe with sufficient accuracy the dislocation structure with a view to modelling the hardening behaviour. Parameters k^s and n^s account for viscosity properties.

4.2.2. Evolution law for the viscoplastic torsion-curvature variables. We consider an array of edge dislocations with $\underline{\mathbf{b}} = b\,\underline{\mathbf{e}}_1$, the normal to the glide plane $\underline{\mathbf{z}} = \underline{\mathbf{e}}_2$ and $\underline{\boldsymbol{\xi}} = -\underline{\mathbf{e}}_3$ (see Fig. 1). At small strains they produce a curvature

$$\underset{\sim}{\boldsymbol{\kappa}}^p = \frac{-nb}{l}\,\underline{\mathbf{e}}_3 \otimes \underline{\mathbf{e}}_1 = \kappa^p_{31}\,\underline{\mathbf{e}}_3 \otimes \underline{\mathbf{e}}_1 \,. \tag{4.9}$$

We will assume that such geometrically necessary dislocations are produced by local dislocation sources if the local moment $\underset{\sim}{\boldsymbol{\mu}} = m\,\underline{\mathbf{e}}_3 \otimes \underline{\mathbf{e}}_1$ ($m < 0$ here) is so high that the imposed curvature cannot be accommodated elastically any longer.

Generalizing the previous example, we propose the following expression of the viscoplastic curvature rate

$$\dot{\theta}^s = \left(\frac{\mathrm{Max}\,(0,\ |{}^\sharp\underset{\sim}{\boldsymbol{\mu}} : {}^\sharp\underset{\sim}{\mathbf{Q}}^s| - l\,r_c^s)}{l\,k_c^s} \right)^{n_c^s} \mathrm{sign}\,({}^\sharp\underset{\sim}{\boldsymbol{\mu}} : {}^\sharp\underset{\sim}{\mathbf{Q}}^s), \tag{4.10}$$

where r_c^s denotes the threshold and k_c^s and n_c^s are viscosity parameters. The formula is to be applied successively for edge and screw dislocations belonging to the same system. Equations (4.8) and (4.10) and the hardening rules of the next section close the theory based on multicriteria and associative flow rules. Accordingly, this theory is part of the associative generalized plasticity.

4.3. Expression of the free energy and hardening rules

The key-point of the thermodynamical analysis of a constitutive model for a dissipative system is the choice of the relevant internal variables on which the free energy may depend. We propose such a formulation of the previous model in the linear case for simplicity. In addition to the observable variables: deformation, curvature and temperature ($\underset{\sim}{\mathbf{e}}$, $\underset{\sim}{\boldsymbol{\kappa}}$, T) or equivalently ($\underset{\sim}{\mathbf{e}}^e$, $\underset{\sim}{\boldsymbol{\kappa}}^e$, T), the free energy is assumed to depend on the following internal variables:

- the variables ϱ_S^s, which are similar to the densities of statistically stored dislocations, and which are defined by

$$\dot{\varrho}_S^s = |\dot{\gamma}^s|; \tag{4.11}$$

- the variables ϱ_G^s, which are similar to the densities of geometrically necessary dislocations, and which are defined by

$$\varrho_G^s = \left| \frac{b\,\theta^s}{l} \right|; \tag{4.12}$$

- the kinematic hardening variables α^s.

We postulate then that the free energy is a quadratic form of these variables according to

$$
\begin{aligned}
(4.13)\qquad \varrho\psi(\underset{\sim}{\mathbf{e}}^e, \underset{\sim}{\boldsymbol{\kappa}}^e, T, \alpha^s, \varrho_S^s, \varrho_G^s) = {} & \frac{1}{2}\underset{\sim}{\mathbf{e}}^e : \underset{\approx}{\mathbf{E}} : \underset{\sim}{\mathbf{e}}^e + \frac{1}{2}\underset{\sim}{\boldsymbol{\kappa}}^e : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\boldsymbol{\kappa}}^e + \frac{1}{2}\sum_{s\in S} c\,\alpha^{s2} \\
& + r_0 \sum_{s\in S} \varrho_S^s + \frac{1}{2}\sum_{r,s\in S} h^{sr}\,\varrho_S^s\,\varrho_S^r \\
& + r_{c0} \sum_{s\in S} \varrho_G^s + \frac{1}{2}\sum_{r,s\in S} h_c^{sr}\,\varrho_G^s\,\varrho_G^r \\
& + \sum_{r,s\in S} h_I^{sr}\,\varrho_S^s\,\varrho_G^r + f(T).
\end{aligned}
$$

Hardening matrices h^{rs} and h_c^{rs} have been introduced for each population of dislocations following [55], but a coupling term associated with the matrix h_I^{sr} must be added.

Assuming then that the thermodynamical forces corresponding to the variables ϱ_S^s, ϱ_G^s and α^s, respectively, are r^s, r_c^s and x^s, the following hardening rules are derived:

Isotropic hardening

$$
(4.14)\qquad r^s = \varrho\frac{\partial\psi}{\partial\varrho_S^s} = r_0 + \sum_{r\in S} h^{sr}\,\varrho_S^r + \sum_{r\in S} h_I^{sr}\,\varrho_G^r\,,
$$

$$
(4.15)\qquad r_c^s = \varrho\frac{\partial\psi}{\partial\varrho_G^s} = r_{c0} + \sum_{r\in S} h_c^{sr}\,\varrho_G^r + \sum_{r\in S} h_I^{sr}\,\varrho_S^r\,.
$$

Note that, for simplicity, we have omitted to split the terms $h_c^{sr}\,\varrho_G^r$ into $h_{c\perp}^{sr}\,\varrho_{G\perp}^r + h_{c\odot}^{sr}\,\varrho_{G\odot}^r$ in order to distinguish the contributions of edge and screw dislocations. The same holds for the terms involving matrix h_I^{sr}. Furthermore, a similar thermodynamical formulation can be worked out for nonlinear isotropic hardening [58]. It can be seen that a coupling between plastic deformation and curvature naturally arises from our choice of the free energy. The existence of additional hardening due to plastic curvature must be investigated experimentally.

Kinematic hardening

$$
(4.16)\qquad x^s = \varrho\frac{\partial\psi}{\partial\alpha^s} = c\,\alpha^s\,.
$$

We refer to [45] for the expression of the nonlinear evolution law for kinematic hardening:

$$
(4.17)\qquad \dot{\alpha}^s = \dot{\gamma}^s - d\,|\dot{\gamma}^s|\alpha^s\,.
$$

4.4. Dissipation

Introducing now the internal variables in the expression of the intrinsic dissipation rate derived in (2.5), one obtains

$$\dot{D} = \sum_{r\in S} \left(\tau^s \dot{\gamma}^s - x^s \dot{\alpha}^s - r^s \dot{\varrho}^s_S + \nu^s_\perp \dot{\theta}^s_\perp + \nu^s_\odot \dot{\theta}^s_\odot - r^s_{c\perp} \dot{\varrho}^s_{G\perp} - r^s_{c\odot} \dot{\varrho}^s_{G\odot} \right), \tag{4.18}$$

where

$$\nu^s_\perp = \frac{1}{l}\, {}^\sharp\underset{\sim}{\boldsymbol{\mu}} : {}^\sharp\underset{\sim}{\mathbf{Q}}^s_\perp \qquad \text{and} \qquad \nu^s_\odot = \frac{1}{l}\, {}^\sharp\underset{\sim}{\boldsymbol{\mu}} : {}^\sharp\underset{\sim}{\mathbf{Q}}^s_\odot . \tag{4.19}$$

The multiplication and motion of dislocations are dissipative processes. The three first terms in (4.18) account for dissipation due to slip activity whereas the remaining terms account for multiplication of geometrically necessary dislocations. In some cases the last terms can be neglected. But when strong lattice rotation gradients develop, they may well be the leading terms.

Some conditions on the material parameters can then be derived from the entropy principle. Taking the flow rules (4.8) and (4.10) and the definitions (4.11) and (4.12) into account, Eq. (4.18) can be rewritten in the form

$$\begin{aligned} \dot{D} = \sum_{r\in S} \Big[& (\tau^s - x^s)\,\mathrm{sign}\,(\dot{\gamma}^s) - r^s + cd\alpha^{s2}|\dot{\gamma}^s| \\ & + \dot{\theta}^s_\perp \left(\nu^s_\perp - r^s_{c\perp}\,\mathrm{sign}\,(\theta^s_\perp)\right) + \dot{\theta}^s_\odot (\nu^s_\odot - r^s_{c\odot}\,\mathrm{sign}\,(\theta^s_\odot)) \Big]. \end{aligned} \tag{4.20}$$

It can be checked in this formula that the positivity of the intrinsic dissipation rate is ensured if $cd > 0$ and if the marix $h^{rs}_{c\perp,\odot}$ is such that $r^s_{c\perp,\odot}$ is always positive.

5. Conclusions

Recent advances in the mechanics of generalized continua have been used to develop a Cosserat theory for single crystals at finite deformation and curvature. The decomposition of the relative deformation gradient into an elastic and plastic part is multiplicative as usual, whereas the wryness tensor admits a mixed additive-multiplicative decomposition. We have assumed that the plastic lattice curvature and torsion are accommodated, respectively, by edge and screw dislocations belonging to each slip system. The curvature and torsion angles over a characteristic length due to each type of dislocation are internal variables in addition to the cumulative amounts of slip for each slip system. Explicit constitutive equations have been proposed in the case of elastoviscoplasticity. An important consequence of the theory is that the plastic lattice curvature and torsion as well as the plastic spin are associated with dissipation. The production of geometrically necessary dislocations is clearly a dissipative process. There

is an overwhelming tendency to include these microstructural features of dislocated crystals into the framework of generalized continua. Since the pioneering work of GÜNTHER [47], CLAUS and ERINGEN [10] resorted to a micromorphic continuum. As for them, SMYSHLAYEV and FLECK [56] prefer to develop a strain gradient theory of slip. However they replace this plasticity problem by a problem of nonlinear elasticity at small strains. In contrast, our theory provides a set of kinematical and constitutive equations in elastoviscoplasticity at finite deformation on a physical and thermodynamical basis. Finally LACHNER *et al.* [57] have shown that polycrystals also can be regarded as Cosserat media. Homogenization techniques should enable one to derive a polycrystal model from the present theory.

Only a precise enough description of dislocation distribution within a volume element can enable one to model the plastic behaviour of single crystals. For that purpose, the continuum theory of dislocations resorts to the dislocation density tensor. In contrast, macroscopic elastoplasticity theory involves hardening variables which are related to scalar dislocation densities. In both theories, the expression "dislocation density" is seen to have a very different meaning. The dislocation density tensor and the scalar dislocation densities are independent measures of the dislocation distribution. The most important advantage of the proposed theory is to combine both descriptions within a single constitutive framework.

It must be noticed that only slip processes have been taken into account in the present work. Further developments are necessary to include climb processes, which may play a significant role during creep.

A coupling between plastic curvature and plastic deformation has been introduced on the level of the hardening rule to represent the influence of slip plane curvature on further dislocation motion. Experimental evidence of such hardening effects have been provided for instance in [59].

It is clear that the difference between the classical theory and the Cosserat theory can appear only if deformation and more precisely, lattice rotation is not homogeneous. The theory can therefore be applied to the prediction and the simulation of localized deformation modes like shear bands in single crystals. A theoretical analysis of such material instabilities is presented in [60], and ASARO and RICE [61] and DUSZEK-PERZYNA and PERZYNA [62] investigate the case of single crystals. An analysis and numerical simulations of localization phenomena in single crystals are presented in [63] for the classical theory. In [58] we have performed a bifurcation analysis for single crystals undergoing single slip using the Cosserat theory. Some crucial differences with respect to the classical case have been pointed out. For instance, according to the classical theory, slip bands and kink bands can occur for the same critical hardening modulus. This is no longer true for the Cosserat theory, which is strongly supported by experimental evidence.

Appendix

Notations

In this work, $\underline{\mathbf{a}}$ denotes a vector of the Euclidean space $\mathbf{E}$, $\underset{\sim}{\mathbf{A}}$ a second-rank Euclidean tensor, and $\underset{\approx}{\mathbf{A}}$ (resp. $\underset{\approx}{\mathbf{A}}$) a third-rank tensor when operating on a vector (resp. a second-rank tensor). The same third-rank tensor is denoted by $\underset{\equiv}{\mathbf{A}}$ when regarded as a 3-linear form. The tensor product of two vectors $\underline{\mathbf{a}}$, $\underline{\mathbf{b}}$ is such that, for all $\underline{\mathbf{x}} \in \mathbf{E}$,

$$\begin{aligned} \underline{\mathbf{x}}\,(\underline{\mathbf{a}} \otimes \underline{\mathbf{b}}) &= \underline{\mathbf{x}} \,.\, \underline{\mathbf{a}}\,\underline{\mathbf{b}}\,, \\ (\underline{\mathbf{a}} \otimes \underline{\mathbf{b}})\,\underline{\mathbf{x}} &= \underline{\mathbf{b}} \,.\, \underline{\mathbf{x}}\,\underline{\mathbf{a}}\,, \end{aligned} \tag{A.1}$$

where the dot denotes the inner product on $\mathbf{E}$.

Let $(\underline{\mathbf{e}}_1, \underline{\mathbf{e}}_2, \underline{\mathbf{e}}_3)$ be a positive oriented orthonormal basis of oriented $\mathbf{E}$ with dimension 3. When written in components, the double contraction of second-rank tensors reads

$$\underset{\sim}{\mathbf{A}} \;:\; \underset{\sim}{\mathbf{B}} = A_{ij}\, B_{ij}\,. \tag{A.2}$$

We note $\underset{\approx}{\epsilon}$ the Levi-Civita tensor

$$\underset{\approx}{\epsilon} = \mathrm{Det}\,(\underline{\mathbf{e}}_j, \underline{\mathbf{e}}_k, \underline{\mathbf{e}}_l)\, \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k \otimes \underline{\mathbf{e}}_l\,. \tag{A.3}$$

Notice the useful identity

$$\epsilon_{ijk}\, \epsilon_{ilm} = \delta_{jl}\, \delta_{km} - \delta_{jm}\, \delta_{kl}\,. \tag{A.4}$$

The following result concerning third-rank tensors have been used,

$$\begin{aligned} &\text{If} \qquad \underset{\sim}{\mathbf{B}} = \frac{1}{2}\, \underset{\approx}{\epsilon} \;:\; \underset{\approx}{\mathbf{A}} = \frac{1}{2} \epsilon_{ikl}\, A_{klj}\, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \\ &\text{and} \qquad A_{ijk} = -A_{jik}\,, \\ &\text{then} \qquad \underset{\approx}{\mathbf{A}} = \underset{\approx}{\epsilon} \,.\, \underset{\sim}{\mathbf{B}} = \epsilon_{ijm}\, B_{mk}\, \underline{\mathbf{e}}_i \otimes \underline{\mathbf{e}}_j \otimes \underline{\mathbf{e}}_k\,. \end{aligned} \tag{A.5}$$

The cross product is defined by

$$\underline{\mathbf{a}} \times \underline{\mathbf{b}} = \underset{\approx}{\epsilon}\,(\underline{\mathbf{a}} \otimes \underline{\mathbf{b}}) = \epsilon_{ijk}\, a_j\, b_k\, \underline{\mathbf{e}}_i\,. \tag{A.6}$$

The symmetric and antisymmetric parts of tensor $\underset{\sim}{\mathbf{A}}$ are respectively denoted $\{\underset{\sim}{\mathbf{A}}\}$ and $\}\underset{\sim}{\mathbf{A}}\{$. There is then one and only one vector $\overset{\times}{\underline{\mathbf{A}}}$ such that, for all $\underline{\mathbf{x}}$,

$$\}\underset{\sim}{\mathbf{A}}\{\,\underline{\mathbf{x}} = \overset{\times}{\underline{\mathbf{A}}} \times \underline{\mathbf{x}} \tag{A.7}$$

and

$$\overset{\times}{\underline{\underline{A}}} = -\frac{1}{2}\underline{\underline{\epsilon}}\,\underline{\underline{A}} = -\frac{1}{2}\epsilon_{klm}\,A_{lm}\,\underline{e}_k\,. \tag{A.8}$$

Following TROSTEL [60], we define a cross product between a second-rank tensor and a vector

$$\begin{aligned}(\underline{a}\otimes\underline{b})\times\underline{c} &= \underline{a}\otimes(\underline{b}\times\underline{c})\,,\\ \underline{a}\times(\underline{b}\otimes\underline{c}) &= (\underline{a}\times\underline{b})\otimes\underline{c}\,,\end{aligned} \tag{A.9}$$

so that

$$\underline{\underline{A}}\times\underline{c} = -(\underline{c}\times\underline{\underline{A}}^T)^T\,. \tag{A.10}$$

As a result

$$\}\underline{\underline{A}}\{ = \underline{\underline{1}}\times\overset{\times}{\underline{\underline{A}}} = -\underline{\underline{\epsilon}}\,\overset{\times}{\underline{\underline{A}}}\,. \tag{A.11}$$

Any element $\underline{\underline{R}}$ of the orthogonal group can be represented by the element $\underline{\Phi}$ of the associated Lie group such that

$$\underline{\underline{R}} = \exp(\underline{\underline{1}}\times\underline{\Phi}) = \exp(-\underline{\underline{\epsilon}}\,\underline{\Phi})\,. \tag{A.12}$$

Concerning tensor analysis, our notations are:

Nabla operator

$$\underline{\nabla} = {}_{,i}\,\underline{e}_i\,, \tag{A.13}$$

gradient operator

$$\underline{\mathrm{grad}}\,f = f\,\underline{\nabla} = f_{,i}\,\underline{e}_i\,, \tag{A.14}$$

$$\underset{\sim}{\mathrm{grad}}\,\underline{u} = \underline{u}\otimes\underline{\nabla} = u_{i,j}\,\underline{e}_i\otimes\underline{e}_j\,, \tag{A.15}$$

curl operator

$$\underline{\mathrm{curl}}\,\underline{u} = \underline{u}\times\underline{\nabla} = \epsilon_{ijk}\,u_{j,k}\,\underline{e}_i\,, \tag{A.16}$$

$$\underset{\sim}{\mathrm{curl}}\,\underline{\underline{A}} = \underline{\underline{A}}\times\underline{\nabla} = \epsilon_{hjk}\,A_{ij,k}\,\underline{e}_i\otimes\underline{e}_h\,. \tag{A.17}$$

Note that

$$\}\underline{u}\otimes\underline{\nabla}\{ = \frac{1}{2}\underline{\underline{\epsilon}}(\underline{\mathrm{curl}}\,\underline{u}). \tag{A.18}$$

We have made a wide use of theorem

$$\oint_L \underline{\underline{A}}\,\underline{l}\;dl = -\int_S(\underset{\sim}{\mathrm{curl}}\,\underline{\underline{A}})\,\underline{n}\;dS\,, \tag{A.19}$$

where the open surface S is bounded by the contour L.

References

1. J. MANDEL, *Equations constitutives et directeurs dans les milieux plastiques et viscoplastiques*, Int. J. Solids Structures, **9**, pp. 725–740, 1973.
2. E. COSSERAT and F. COSSERAT, *Théorie des corps déformables*, Hermann, Paris 1909.
3. J.F. NYE, *Some geometrical relations in dislocated crystals*, Acta Metall., **1**, pp. 153–162, 1953.
4. E. KRÖNER, *On the physical reality of torque stresses in continuum mechanics*, Int. J. Engng. Sci., **1**, pp. 261–278, 1963.
5. F. HEHL and E. KRÖNER, *Zum Materialgesetz eines elastischen Mediums mit Momentenspannungen*, Z. Naturforschg., **20 a**, pp. 336–350, 1965.
6. F.A. MCCLINTOCK, P.A. ANDRÉ, K.R. SCHWERDT and R.E. STOECKLY, *Interface couples in crystals*, Nature, No. 4636, pp. 652–653, 1958.
7. E. KRÖNER, *Mechanics of generalized continua*, Proc. of the IUTAM-Symposium on the Generalized Cosserat Continuum and the Continuum Theory of Dislocations with Applications, Freudenstadt, Springer-Verlag, Stuttgart 1967.
8. S. KESSEL, *Spannungsfelder einer Schraubenversetzung und einer Stufenversetzung im Cosseratschen Kontinuum*, ZAMM, **50**, 9, pp. 547–553, 1970.
9. E. KRÖNER, *A variational principle in nonlinear dislocation theory*, Proc. of the Second International Conference of Nonlinear Mechanics, pp. 59–64, Beijing 1993.
10. W.D. CLAUS and A.C. ERINGEN, *Three dislocation concepts and micromorphic mechanics*, Developments in Mechanics, Vol. 6, Proc. of the 12th Midwestern Mechanics Conference, 1971.
11. CZ. WOŹNIAK, *Thermoelasticity of bodies with micro-structure*, Arch. Mech. Stos., **19**, 3, pp. 335–365, 1966.
12. K. WILMAŃSKI and CZ. WOŹNIAK, *On geometry of continuous medium with micro-structure*, Arch. Mech. Stos., **19**, 5, pp. 715–723, 1967.
13. K.C. LE and H. STUMPF, *Finite elastoplasticity with microstructure*, Mitteilung aus dem Institut für Mechanik der Ruhr-Universität Bochum, No. 92, 1994.
14. K.C. LE and H. STUMPF, *Nonlinear continuum theory of dislocations*, Int. J. Engng. Sci., **34**, 3, pp. 339–358, 1996.
15. C.B. KAFADAR and A.C. ERINGEN, *Micropolar media: I the classical theory*, Int. J. Engng Sci., **9**, pp. 271–305, 1971.
16. P. GERMAIN, *The method of virtual power in continuum mechanics, Part 2: Microstructure*, SIAM, J. Appl. Math., **25**, 3, pp. 556–575, 1973.
17. W. NOWACKI, *Theory of asymmetric elasticity*, (Polish edition, 1977), Pergamon, 1986.
18. S. KESSEL, *Lineare Elastizitätstheorie des anisotropen Cosserat-Kontinuums*, Abhandlungen der Braunschweig. Wiss. Ges., Vol. 16, 1964.
19. A. SAWCZUK, *On yielding of Cosserat continua*, Arch. Mech. Stos., **19**, 3, pp. 471–480, 1967.
20. H. LIPPMANN, *Eine Cosserat-Theorie des plastischen Fließens*, Acta Mech., **8**, pp. 255–284, 1969.

21. D. BESDO, *Ein Beitrag zur nichtlinearen Theorie des Cosserat-Kontinuums*, Acta Mech., **20**, pp. 105–131, 1974.

22. R. SIEVERT, *Eine Systematik für elastisch-plastische Stoffgleichungen*, Dissertation, Schriftenreihe Phys. Ing.-Wiss., Band 23, TU Berlin 1992.

23. J. MANDEL, *Plasticité classique et viscoplasticité*, CISM, Udine, Springer Verlag, 1971.

24. P. STEINMANN, *A micropolar theory of finite deformation and finite rotation multiplicative elastoplasticity*, Int. J. Solids Struct., **31**, pp. 1063–1084, 1994.

25. P.H. DŁUŻEWSKI, *Finite deformations of polar media in angular coordinates*, Arch. Mech., **43**, 6, pp. 783–793, 1991.

26. C. SANSOUR and J. KECK, *Zum elasto-viskoplastischen Cosserat-Kontiuum*, Mitteilungen aus dem Institut für Mechanik der Ruhr-Universität Bochum, FRG, No. 93, pp. 38–41, 1994.

27. C. TEODOSIU, *A dynamic theory of dislocations and its applications to the theory of the elastic-plastic continuum*, [in:] Fundamental Aspects of Dislocation Theory, J.A. SIMMONS, R. DE WIT, R. BULLOUGH [Eds.], Nat. Bur. Stand. (U.S.), Spec. Pub., 317, Vol. II, 1970.

28. E. KRÖNER, *Kontinuumstheorie der Versetzungen und Eigenspannungen*, Ergebnisse der angewanden Mathematik, Vol. 5, Springer-Verlag, 1958.

29. E. KRÖNER and C. TEODOSIU, *Lattice defect approach to plasticity and viscoplasticity*, [in:] Problems of Plasticity, International Symposium on Foundations of Plasticity, Warsaw, A. SAWCZUK [Ed.], Noordhoff International Publishing, Leyden 1972.

30. T. MURA, *On dynamic problems of continuous distribution of dislocations*, Int. J. Engng. Sci., **1**, pp. 371–381, 1963.

31. T. MURA, *Continuous distribution of moving dislocations*, Philosophical Magazine, **8**, 89, pp. 843–857, 1963.

32. J.P. HIRTH and J. LOTHE, *Theory of dislocations*, Wiley-Interscience, 1982.

33. E. KOSSECKA and R. DE WIT, *Disclination kinematics*, Arch. Mech., **29**, 5, pp. 633–651, 1977.

34. H.T. HAHN and W. JAUNZEMIS, *A dislocation theory of plasticity*, Int. J. Engng. Sci., **11**, pp. 1065–1078, 1973.

35. T. MURA, *Continuous distribution of dislocations and the mathematical theory of plasticity*, Phys. Stat. Sol., **10**, pp. 447–453, 1965.

36. R.W. LARDNER, *Dislocation dynamics and the theory of the plasticity of single crystals*, ZAMP, **20**, pp. 514–529, 1969.

37. M. EISENBERG, *On the relation between continuum plasticity and dislocation theories*, Int. J. Engng. Sci., **8**, pp. 261–271, 1970.

38. H. ZORSKI, *Statistical theory of dislocations*, Int. J. Solids Structures, **4**, pp. 959–974, 1968.

39. E. KRÖNER, *Initial studies of a plasticity theory based upon statistical mechanics*, Inelastic Behaviour of Solids, M.F. KANNINEN, W.F. ADLER, A.R. ROSENFIELD, R.I. JAFFEE, McGraw-Hill, 1969.

40. B.A. BILBY, R. BULLOUGH, L.R.T. GARDNER and E. SMITH, *Continuous distributions of dislocations IV: Single glide and plane strain*, Proc. Roy. Soc., **A 236**, pp. 538–557, 1957.

41. J. ZARKA, *Généralisation de la théorie du potentiel plastique multiple en viscoplasticité*, J. Mech. Phys. Solids, **20**, 3, pp. 179–195, 1972.

42. C. TEODOSIU and F. SIDOROFF, *A theory of finite elastoviscoplasticity of single crystals*, Int. J. Engng. Sci., **14**, pp. 713–723, 1976.

43. R. FORTUNIER, *Contribution à l'étude de la déformation plastique des cristaux et des polycristaux*, thesis, Ecole des Mines de Saint-Etienne, 1987.

44. G. CAILLETAUD, *A micromechanical approach to inelastic behavior*, Int. J. Plasticity, **8**, pp. 55–73, 1992.

45. L. MÉRIC, P. POUBANNE and G. CAILLETAUD, *Single crystal modeling for structural calculations. Part 1. Model presentation*, J. Engng. Materials and Technology, **113**, pp. 162–170, 1991.

46. P. DŁUŻEWSKI, *On geometry and continuum thermodynamics of movement of structural defects*, Mech. of Materials, **22**, pp. 23–41, 1996.

47. W. GÜNTHER, *Zur Statik und Kinematik des Cosseratschen Kontinuums*, Abhandlungen der Braunschweig. Wiss. Ges., **10**, pp. 195–213, 1958.

48. H. SCHÄFER, *Das Cosserat-Kontinuum*, ZAMM, **47**, 8, pp. 485–498, 1967.

49. M.F. ASHBY, *The deformation of plastically non-homogeneous alloys*, [in:] Strengthening Methods in Crystals, A. KELLY and R.B. NICHOLSON [Eds.], Applied Science Publishers, London, pp. 137–192, 1971.

50. N.A. FLECK, G.M. MÜLLER, M.F. ASHBY and J.W. HUTCHINSON, *Strain gradient plasticity: theory and experiment*, Acta Metall. Mater., **42**, 2, pp. 475–487, 1994.

51. R. DE BORST, *A generalization of J_2-flow theory for polar continua*, Computer Methods in Appl. Mech. and Engng., **103**, pp. 347–362, 1993.

52. P.H. DŁUŻEWSKI, *Finite elastic-plastic deformations of oriented media*, MECAMAT'92, Int. Seminar on Multiaxial Plasticity, A. Benallal, R. Billardon, D. Marquis, Laboratoire de Mécanique et Technologie, Cachan, France, pp. 668–688, 1993.

53. J. FRIEDEL, *Dislocations*, Pergamon, 1964.

54. E. KRÖNER, *Die Versetzung als elementare Eigenspannungsquelle*, Z. Naturforschg., **11a**, pp. 969–985, 1956.

55. J. MANDEL, *Généralisation de la théorie de la plasticité de W.T. Koiter*, Int. J. Solids Structures, **1**, pp. 273–295, 1965.

56. V.P. SMYSHLYAEV and N.A. FLECK, *The role of strain gradients in the grain size effect for polycrystals*, J. Mech. Phys. Solids, pp. 465–495, 1996.

57. D. LACHNER, H. LIPPMANN and L.S. TÓTH, *On Cosserat plasticity and plastic spin for isotropic materials*, Arch. Mech., **46**, 4, pp. 534–539, 1994.

58. S. FOREST, *Mechanical modelling of non-homogeneous deformation of single crystals*, Doctoral Thesis, ENSMP, Paris 1996.

59. B. JAOUL, *Influence de la sous-structure de monocristaux d'aluminium sur la forme des courbes de déformation plastique*, C.R. Acad. Sci. Paris, Vol. 242, pp. 2372–2374, 1956.

60. H. PETRYK, *Material instability and strain-rate discontinuities in incrementally nonlinear continua*, J. Mech. Phys. Solids, **40**, 6, pp. 1227–1250, 1992.

61. R.J. ASARO and J.R. RICE, *Strain localization in ductile single crystals*, J. Mech. Phys. Solids, **25**, pp. 309–338, 1977.

62. M. DUSZEK-PERZYNA and P. PERZYNA, *Adiabatic shear band localization in elastic-plastic single crystals*, Int. J. Solids Structures, **30**, 1, pp. 61–89, 1993.

63. S. FOREST and G. CAILLETAUD, *Strain localization in single crystals: effect of boundaries and interfaces*, Eur. J. Mech., A/Solids, **14**, 5, pp. 747–771, 1995.

64. R. TROSTEL, *Vektor- und Tensor-Algebra*, Mathematische Grundlagen der technischen Mechanik I, Beiträge zur theoretische Mechanik, Vieweg, Wiesbaden 1993.

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