- The cohesive strength, the work of separation and thus the cohesive characteristic length of the cohesive zone are being determined within the crack growth simulation. There is no need to perform an a priori choice of the cohesive zone parameters once their dependence on the triaxiality is known from e.g. micromechanical considerations.
- The new model can reflect the effects of changing triaxiality on material separation with increasing crack growth. It predicts different traction separation curves for points close to and more distant from the initial crack tip. The maximum stress at the crack tip is increased and the lengthscale of the separation process is decreased as the crack propagates, Fig. 7.

With respect to these two items the triaxiality dependent cohesive zone model provides results that are in – at least qualitative – agreement with the predictions from the application of the Gurson model to the crack growth simulation. The new cohesive zone model is thus a promising tool for the investigation of the effects of changing constraint as imposed by a variation in the size and geometry of fracture mechanics specimen.

Acknowledgment: The authors want to thank E. van der Giessen, TU-Delft, NL, for the discussion on the subject.

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Finite deformation Cosserat-type modelling of dissipative solids and its application to crystal plasticity

R. Sievert, S. Forest* and R. Trostel**

Bundesanstalt für Materialforschung und –prüfung (BAM), Unter den Eichen 87, 12200 Berlin, Germany
** École des Mines de Paris, Centre des Matériaux, UMR 7633 du CNRS, BP. 87, 91003 Evry, France*
*** Techn. Univ. Berlin, Inst. für Mechanik (FB 10), 10623 Berlin, Germany*

Abstract : Recently, several proposals were made for the enlargement of the classical field equations in order to solve locally inhomogeneous deformation problems (e.g. at shear banding and damage localization or of composites). In the present paper basic issues of this topic will be treated : i) the implicit dependence within the gradient plasticity theory, ii) the more open micromorphic view-point of the gradient of internal variable approach, iii) a derivation of an elastic-plastic decomposition of the Cosserat strain measures, iv) its application to the description of lattice curvature in crystals. Finally, finite element simulations of strain localization in Cosserat single crystals are presented.

1. INTRODUCTION

When the size of a macroscopic structure is not so far from the relevant substructural scale, then a material element of a continuum theory can not be considered as so small because of its resolution limit. On the other hand, if one imagines an element as larger, the local movement within that can be described no more in the classical way, i.e. by the linear approximation on the basis of the macroscopic displacement, only. In order to take into account nevertheless *structured local movements* (as lattice rotations or damage formations) in a *field theory*, a systematic way to enrich the classical continuum is the introduction of *additional kinematical degrees of freedom*, i.e. an internal rotation or internal strains (see also [1,2]), and of higher-order gradients of the degrees of freedom, e.g. the second gradient of displacement. If local movements can be identified within a material, then strains or strain rates of these kinematical variables have to be supposed in principle as energetically effective (e.g. dissipative). Further, if the fundamental relations of thermodynamics for a body, i.e. the energy conservation law and the dissipation inequality, are fulfilled identically, then also a power of contact which is generalized by gradients of velocities can be considered as thermodynamically admissible.

An elastic-plastic decomposition of the rotation, as of the displacement, is not recommendable, because these non-objective variables cannot be connected with the quantities *energy* and *dissipation*. Such a connection is possible only on the level of strains. One possible elastic-plastic decomposition of the curvature-torsion tensor is proposed that turns out to be the appropriate tool to explicitely model lattice curvature in crystal plasticity. The physical basis of such an extension of Mandel's classical framework [3] is recalled and an application in the case of localized deformation in single crystals is provided in section 5.

Starting point are the following basic energetic relations: The power balance of mechanics for a body in a quasi-static process (no storage of kinetic energy) is : $\mathcal{P}_c + \mathcal{P}_e = \mathcal{P}_i$, where $\mathcal{P}_c$ denotes the *power of contact*, $\mathcal{P}_e$ the *external power* and $\mathcal{P}_i$ the internal power, i.e. the *power of deformation*. The dissipation inequality of mechanics says that $\mathcal{P}_i$ is always greater than the power stored as energy $\Psi = \int_\mathcal{V} \psi \rho dV$: $\mathcal{D} := \mathcal{P}_i - \dot{\Psi} \geq 0$. $\mathcal{D} = \int_\mathcal{V} d\rho dV$ denotes the *dissipation power* (ρ mass density). Strain-energy ψ can be stored **also without** d : this gives the *strain-energy of elasticity* ψ_e. Thus, the remainder of ψ can be stored **only** together **with** d : this is the *plastic strain-energy* $\psi_p := \psi - \psi_e$. Hence, the power balance reads as $\mathcal{P}_c + \mathcal{P}_e = \dot{\Psi}_e + \dot{\Psi}_p + \mathcal{D}$.

For tensor algebra and analysis, also for higher-order continua, see [4].

2. CONJUGATE VARIABLES AT DIFFERENT DEPENDENCIES ON STRAIN-GRADIENTS

In order to point out the basic mathematical structure of the problem, this section is restricted to small deformations.

2.1. Cosserat continua also sensitive to the second gradient of displacement

The strain measures are the first gradient of the displacement $\underline{\mathbf{u}}$ relative to the internal rotation $\underline{\mathbf{\Phi}}$, i.e. $\underline{\mathbf{u}} \otimes \underline{\nabla} - \underline{\mathbf{\Phi}} \times \underline{\mathbf{1}}$, as well as preliminarily the second gradient of displacement $\underline{\mathbf{u}} \otimes \underline{\nabla} \otimes \underline{\nabla}$ and the curvature-torsion strain $\underline{\mathbf{\Phi}} \otimes \nabla$ (for sandwich or beam structures cf. [5,6], respectively). Using Toupin's reduction of the gradient of the mean rotation of the displacement field

$$\tfrac{1}{2}\underline{\nabla} \times \underline{\mathbf{u}} \otimes \underline{\nabla} = \tfrac{1}{2}\underline{\nabla} \times (\underline{\nabla} \otimes \underline{\mathbf{u}} + \underline{\mathbf{u}} \otimes \underline{\nabla}) = \underline{\nabla} \times \underline{\mathbf{1}}.^{\{}\underline{\mathbf{u}} \otimes \underline{\nabla}\} = \underline{\mathbf{1}} \times \underline{\mathbf{1}}..\underline{\nabla} \otimes {}^{\{}\underline{\mathbf{u}} \otimes \underline{\nabla}\} \tag{1}$$

the gradient fields $\underline{\mathbf{u}} \otimes \underline{\nabla} \otimes \underline{\nabla}$ and $\underline{\mathbf{\Phi}} \otimes \underline{\nabla} = -(\tfrac{1}{2}\underline{\nabla} \times \underline{\mathbf{u}} - \underline{\mathbf{\Phi}}) \otimes \underline{\nabla} + \tfrac{1}{2}\underline{\nabla} \times \underline{\mathbf{u}} \otimes \underline{\nabla}$ can be reduced to $({}^{\{}\underline{\mathbf{u}} \otimes \underline{\nabla}\} + (\tfrac{1}{2}\underline{\nabla} \times \underline{\mathbf{u}} - \underline{\mathbf{\Phi}}) \times \underline{\mathbf{1}}) \otimes \underline{\nabla}$. Thus equivalent strain measures are : $\underline{\mathbf{u}} \otimes \underline{\nabla} - \underline{\mathbf{\Phi}} \times \underline{\mathbf{1}} =: \underset{\sim}{\mathbf{Z}} \equiv {}^{\{}\underline{\mathbf{u}} \otimes \underline{\nabla}\} + (\tfrac{1}{2}\underline{\nabla} \times \underline{\mathbf{u}} - \underline{\mathbf{\Phi}}) \times \underline{\mathbf{1}})$ and $\underset{\sim}{\mathbf{Z}} \otimes \underline{\nabla}$. For continua sensitive to these strains, the equilibrium equations and the representation of the power of contact (boundary conditions of [7], cf. [8] with regard to dissipative behaviour, too) have been given in [9] (with regard to laminates).

The elastic-plastic decomposition of a small strain is clear : $\underset{\sim}{\mathbf{Z}} = \underset{\sim}{\mathbf{Z}}_e + \underset{\sim}{\mathbf{Z}}_p$. This implies the decomposition $\underset{\sim}{\mathbf{Z}} \otimes \underline{\nabla} = \underset{\sim}{\mathbf{Z}}_e \otimes \underline{\nabla} + \underset{\sim}{\mathbf{Z}}_p \otimes \underline{\nabla}$. Thus, also the plastic part of $\underset{\sim}{\mathbf{Z}} \otimes \underline{\nabla}$ has the gradient structure and $\underset{\sim}{\mathbf{Z}}_p$ is the **elementary field** also in a gradient plasticity problem.

After separation of the hyperelastic constitutive equations for the stresses, the local dissipation power d is for vanishing energy storage due to hardening equal to the plastic power of deformation :

$$d = (\underline{\underline{\mathbf{S}}}/\rho)..\dot{\underset{\sim}{\mathbf{Z}}}_p^T + (\underline{\underline{\underline{\mathbf{S}}}}/\rho)...(\underline{\nabla} \otimes \dot{\underset{\sim}{\mathbf{Z}}}_p^T).$$

Analogously to the first integration by parts at the derivation of the balance equations, the dissipation inequality is rewritten :

$$\rho d = \dot{\underset{\sim}{\mathbf{Z}}}_p^T..\underline{\underline{\mathbf{S}}} - \dot{\underset{\sim}{\mathbf{Z}}}_p^T..(\underline{\underline{\underline{\mathbf{S}}}}.\underline{\nabla}) + (\dot{\underset{\sim}{\mathbf{Z}}}_p^T..\underline{\underline{\underline{\mathbf{S}}}}).\underline{\nabla} \geq 0, \quad \mathcal{D} = \int_{\mathcal{V}} \dot{\underset{\sim}{\mathbf{Z}}}_p^T..(\underline{\underline{\mathbf{S}}} - \underline{\underline{\underline{\mathbf{S}}}}.\underline{\nabla})dV + \int_{\partial\mathcal{V}} \dot{\underset{\sim}{\mathbf{Z}}}_p^T..\underline{\underline{\underline{\mathbf{S}}}}.\underline{\mathbf{n}}dA \geq 0. \tag{2}$$

In order to fulfill this, $\dot{\underset{\sim}{\mathbf{Z}}}_p$ and its conjugate stress should have a certain dependence at each point in the volume of the body, and also the integrand of the surface integral should be non-negative at each point on the surface. Because the conjugate or effective stress quantity depends on a (second) space-derivative (of $\underset{\sim}{\mathbf{Z}}_e$), equation (2)b reveals that $\underset{\sim}{\mathbf{Z}}_p$ is in principle the solution of an initial boundary-value problem in a gradient plasticity theory. The integrand of the surface integral gives the boundary conditions. For Maxwell-type behaviour $\dot{\underset{\sim}{\mathbf{Z}}}_p$ could be set, in the sense of a sufficient condition, simply proportional to the effective stress :

$$\dot{\underset{\sim}{\mathbf{Z}}}_p = f(||\underline{\underline{\mathbf{S}}}||)\underset{\sim}{\mathbf{A}}..(\underline{\underline{\mathbf{S}}} - \underline{\underline{\underline{\mathbf{S}}}}.\underline{\nabla}). \tag{3}$$

If the strain-energy of elasticity does not depend on the strain-gradient $\underset{\sim}{\mathbf{Z}}_e \otimes \underline{\nabla}$, then only the classical symmetric tensors remain relevant, ${}^{\{}\underline{\mathbf{u}} \otimes \underline{\nabla}\} =: \underline{\underline{\varepsilon}}$. Nevertheless, at a dependence of the plastic strain-energy ψ_p (per unit mass) on the gradient of the accumulated plastic strain p the remaining dissipation inequality has the representation :

$$\mathcal{D} = \int_{\mathcal{V}} \left[\underline{\underline{\mathbf{S}}}..\dot{\underline{\underline{\varepsilon}}}_p^{\star} + \underline{\nabla}.(\rho\frac{d\hat{\psi}_p}{d\underline{\nabla}p})\right]\dot{p}dV - \int_{\partial\mathcal{V}} \underline{\mathbf{n}}.\rho\frac{d\hat{\psi}_p}{d\underline{\nabla}p}\dot{p}dA \geq 0, \quad \text{with} \quad \dot{\underline{\underline{\varepsilon}}}_p^{\star} := \frac{\dot{\underline{\underline{\varepsilon}}}_p}{\dot{p}}. \tag{4}$$

One approach to fulfill that is the use of a *yield condition for the effective stress* of equation (4) (for Mises-type behaviour see equation (99) in [10]) : a quadratic dependence of ψ_p on $\underline{\nabla}p$ reads for isotropic or cubic behaviour (note that also the cubic heat conduction is isotropic) as $\hat{\psi}_p(\underline{\nabla}p) = \frac{1}{2}\frac{k}{\rho}(\underline{\nabla}p)^2$. An approach where energy is stored with a gradient of an internal strain-variable is similar to that of the micromorphic theory (e.g. [11]). This line will be traced in the next section.

2.2. Continua also sensitive to a micromorphic internal variable

The external power and the power of contact respectively are,

$$\mathcal{P}_e = \int_{\mathcal{V}} (\underline{\mathbf{f}}.\dot{\underline{\mathbf{u}}} + ... + y\dot{\beta})dV, \quad \mathcal{P}_c = \int_{\partial\mathcal{V}} (\dot{\underline{\mathbf{u}}}.\underline{\underline{\mathbf{S}}}.\underline{\mathbf{n}} + ... + \dot{\beta}\underline{\mathbf{b}}.\underline{\mathbf{n}})dA. \tag{5}$$

The power balance reads then as $\int_{\mathcal{V}}(...).\dot{\underline{\mathbf{u}}} + ... + (y + \underline{\nabla}.\underline{\mathbf{b}})\dot{\beta}dV = \dot{\Psi}_e + \dot{\Psi}_p + \mathcal{D} - \int_{\mathcal{V}}(... + \underline{\mathbf{b}}.\underline{\nabla}\dot{\beta})dV$. Here, the dotted ranges indicate the balances of equilibrium and the representation of the power of deformation of the classical (Cosserat) continuum, respectively. Setting the brackets of the classical balances identically zero, the dissipation power is

$$\mathcal{D} = \int_{\mathcal{V}} (y + \underline{\nabla}.\underline{\mathbf{b}})\dot{\beta}dV + \int_{\mathcal{V}} (... + \underline{\mathbf{b}}.\underline{\nabla}\dot{\beta})dV - \int_{\mathcal{V}} (\dot{\psi}_e + \dot{\psi}_p)\rho dV \geq 0, \tag{6}$$

β can be a *variable of loss of strength*, i.e. a softening or damage variable (e.g. a void fraction). For the sake of simplicity, it is assumed that only ψ_p depends on the internal variable β, and that on $\underline{\nabla}\beta$ only. After separation of the hyperelastic equations for the classical (Cosserat) stresses depending on ψ_e, the remaining last two terms of (6) give a representation of the micromorphic stress vector : $\underline{\mathbf{b}} = \rho d\hat{\psi}_p/d\underline{\nabla}\beta$. In order to fulfill the inequality (6) at the first term, $\dot{\beta}$ can be set proportional to its conjugate force. As mentioned above, the quadratic dependence of ψ_p on $\underline{\nabla}\beta$ reads for isotropic or cubic behaviour as $\hat{\psi}_p(\underline{\nabla}\beta) = \frac{1}{2}\frac{k}{\rho}(\underline{\nabla}\beta)^2$. Then the resulting equation is

$$c\dot{\beta} = y + k\Delta\beta, \quad \text{with} \quad \Delta := \underline{\nabla}.\underline{\nabla}. \tag{7}$$

The necessary additional boundary conditions for that are given by the last term of the power of contact (5)b. The external force y can be **any** functions of β or, e.g., of the classical stresses [12]. This possible nonlinear dependence of the driving force y on the classical stresses (e.g. the sinh of the Gurson model) represents a more general approach than that based only on the power of deformation (section 2.1) which is inevitably linear in stress. Nevertheless, equation (7) is a more linear problem than the equation (3).

An equation of the type (7) has been applied in [13] to rate-dependent damaging behaviour (of concrete). No mesh-dependence was observed. For rate-independent behaviour, the parameter c depends homogeneously of degree 1 on the reciprocal of an equivalent plastic strain rate.

3. ELASTIC-PLASTIC DECOMPOSITION OF THE COSSERAT STRAIN MEASURES AT LARGE DEFORMATION

Dissipative materials are considered which can behave purely elastically in the current configuration (as metals). This gives rise to the assumption that only parts of the total strains determine the strain-energy of elasticity, called *elastic* parts of strains :

$$\psi_e = \hat{\psi}_e({}^{\sharp}\underset{\sim}{\mathbf{F}}_e, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e, \underset{\sim}{\alpha}_e) \begin{cases} > 0, if({}^{\sharp}\underset{\sim}{\mathbf{F}}_e, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e) \neq (\underline{\mathbf{1}}, \underline{\underline{\mathbf{0}}}) \\ = 0, if({}^{\sharp}\underset{\sim}{\mathbf{F}}_e, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e) = (\underline{\mathbf{1}}, \underline{\underline{\mathbf{0}}}) \end{cases} \tag{8}$$

$\underset{\sim}{\alpha}_e$ are elastic stiffness variables with the same transformation properties as the observer- invariant total strains : ${}^{\sharp}\underset{\sim}{\mathbf{F}} := \underline{\underline{\mathbf{R}}}^T{}^{\sharp}\underset{\sim}{\mathbf{F}}$, ${}^{\sharp}\underline{\underline{\mathbf{\Gamma}}} := \underline{\underline{\mathbf{R}}}^T{}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}$, $\underline{\underline{\mathbf{R}}}$ internal rotation, ${}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}$ curvature-torsion strain (wryness [11], cf [14]). The internal variables $\underset{\sim}{\alpha}_e$ can describe changes of elastic stiffness or elastic symmetry. In the simplest case of the conservation of elastic properties, the elastic constitutive function does not depend on $\underset{\sim}{\alpha}_e$ (called isomorphic elastic behaviour in [15,16]). The elastic parts of strains can arise also without dissipation power. Thus, the remainders of the total strains can evolve only together with dissipation power, these are the *plastic* parts of strains. This elastic-plastic decomposition is represented in such a way, that the total strains are set as general constitutive functions of their parts [17], which have the same transformation properties as the total strains :

$${}^{\sharp}\underset{\sim}{\mathbf{F}} = {}^{\sharp}\hat{\underset{\sim}{\mathbf{F}}}({}^{\sharp}\underset{\sim}{\mathbf{F}}_e, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e, {}^{\sharp}\underset{\sim}{\mathbf{F}}_p, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_p) \quad \text{and} \quad {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}} = {}^{\sharp}\hat{\underline{\underline{\mathbf{\Gamma}}}}({}^{\sharp}\underset{\sim}{\mathbf{F}}_e, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e, {}^{\sharp}\underset{\sim}{\mathbf{F}}_p, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_p). \tag{9}$$

These strain-functions are (mathematically) isotropic. They obey the following conditions :

$${}^{\sharp}\hat{\underset{\sim}{\mathbf{F}}}({}^{\sharp}\underset{\sim}{\mathbf{F}}_e = \underline{\mathbf{1}}, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e, {}^{\sharp}\underset{\sim}{\mathbf{F}}_p = \underline{\mathbf{1}}, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_p) \equiv \underline{\mathbf{1}}, \quad {}^{\sharp}\hat{\underline{\underline{\mathbf{\Gamma}}}}({}^{\sharp}\underset{\sim}{\mathbf{F}}_e, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_e = \underline{\underline{\mathbf{0}}}, {}^{\sharp}\underset{\sim}{\mathbf{F}}_p, {}^{\sharp}\underline{\underline{\mathbf{\Gamma}}}_p = \underline{\underline{\mathbf{0}}}) \equiv \underline{\underline{\mathbf{0}}}$$

$$ {}^{t}\hat{\underset{\sim}{F}}({}^{t}\underset{\sim}{F}_e,\ {}^{t}\underset{\sim}{\Gamma}_e,\ {}^{t}\underset{\sim}{F}_p=\underset{\approx}{1},\ {}^{t}\underset{\sim}{\Gamma}_p=\underset{\sim}{0})\equiv {}^{t}\underset{\sim}{F}_e, \quad {}^{t}\hat{\underset{\sim}{\Gamma}}({}^{t}\underset{\sim}{F}_e,\ {}^{t}\underset{\sim}{\Gamma}_e,\ {}^{t}\underset{\sim}{F}_p=\underset{\approx}{1},\ {}^{t}\underset{\sim}{\Gamma}_p=\underset{\sim}{0})\equiv {}^{t}\underset{\sim}{\Gamma}_e $$

$$ {}^{t}\hat{\underset{\sim}{F}}({}^{t}\underset{\sim}{F}_e=\underset{\approx}{1},\ {}^{t}\underset{\sim}{\Gamma}_e=\underset{\sim}{0},\ {}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)\equiv {}^{t}\underset{\sim}{F}_p, \quad {}^{t}\hat{\underset{\sim}{\Gamma}}({}^{t}\underset{\sim}{F}_e=\underset{\approx}{1},\ {}^{t}\underset{\sim}{\Gamma}_e=\underset{\sim}{0},\ {}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)\equiv {}^{t}\underset{\sim}{\Gamma}_p. \qquad (10) $$

The local dissipation inequality of classical Cosserat continua at large deformation is

$$ \rho d = {}^{t}\underset{\sim}{\sigma}..({}^{t}\dot{\underset{\sim}{F}}\,{}^{t}\underset{\sim}{F}^{-1})^T + {}^{t}\underset{\sim}{\mu}..({}^{t}\dot{\underset{\sim}{\Gamma}}\,{}^{t}\underset{\sim}{F}^{-1})^T - \rho\dot{\psi} \geq 0, \quad \text{with} \quad {}^{t}\underset{\sim}{\sigma} := \underset{\sim}{R}^T\underset{\sim}{\sigma}\underset{\sim}{R},\ {}^{t}\underset{\sim}{\mu} := \underset{\sim}{R}^T\underset{\sim}{\mu}\underset{\sim}{R} \qquad (11) $$

with the Cauchy force- and couple-stress $\underset{\sim}{\sigma}$ and $\underset{\sim}{\mu}$, respectively. At a dependence of the strain functions ${}^{t}\hat{\underset{\sim}{F}}$ and ${}^{t}\hat{\underset{\sim}{\Gamma}}$ only on the corresponding elastic parts (besides the plastic ones), substitution into the inequality gives the hyperelastic constitutive equations for the relative Eulerian stresses in a general form :

$$ {}^{t}\underset{\sim}{\sigma} = \rho\frac{\partial\hat{\psi}_e}{\partial\,{}^{t}\underset{\sim}{F}_e}..(\frac{\partial\,{}^{t}\hat{\underset{\sim}{F}}^T}{\partial\,{}^{t}\underset{\sim}{F}_e})^{-1}\,{}^{t}\underset{\sim}{F}^T \quad \text{and} \quad {}^{t}\underset{\sim}{\mu} = \rho\frac{\partial\hat{\psi}_e}{\partial\,{}^{t}\underset{\sim}{\Gamma}_e}..(\frac{\partial\,{}^{t}\hat{\underset{\sim}{\Gamma}}^T}{\partial\,{}^{t}\underset{\sim}{\Gamma}_e})^{-1}\,{}^{t}\underset{\sim}{F}^T. \qquad (12) $$

In the pure hyperelastic case, with ${}^{t}\underset{\sim}{F} \equiv {}^{t}\underset{\sim}{F}_e$ and ${}^{t}\underset{\sim}{\Gamma} \equiv {}^{t}\underset{\sim}{\Gamma}_e$, these relations read ${}^{t}\underset{\sim}{\sigma} = \rho\frac{\partial\hat{\psi}_e}{\partial\,{}^{t}\underset{\sim}{F}}\,{}^{t}\underset{\sim}{F}^T$, and ${}^{t}\underset{\sim}{\mu} = \rho\frac{\partial\hat{\psi}_e}{\partial\,{}^{t}\underset{\sim}{\Gamma}}\,{}^{t}\underset{\sim}{F}^T$. The question is : What are the representations of the elastic strains depending on the total and plastic ones? For the *partially pure elastic materials* under consideration the most natural assumption is that the elastic equations for the Eulerian stresses still have the **same form** in $\hat{\psi}_e$ as well as in elastic strain measures as in the pure hyperelastic case :

$$ {}^{t}\underset{\sim}{\sigma} = \rho\frac{\partial\hat{\psi}_e}{\partial\,{}^{t}\underset{\sim}{F}_e}\,{}^{t}\underset{\sim}{F}_e^T, \quad \text{and} \quad {}^{t}\underset{\sim}{\mu} = \rho\frac{\partial\hat{\psi}_e}{\partial\,{}^{t}\underset{\sim}{\Gamma}_e}\,{}^{t}\underset{\sim}{F}_e^T, \qquad (13) $$

Then, setting the special constitutive relations (13) equal to the general hyperelastic forms (12) and fulfilling that by one decomposition of strain (${}^{t}\hat{\underset{\sim}{F}}$, ${}^{t}\hat{\underset{\sim}{\Gamma}}$) for any material ($\hat{\psi}_e$) of the class (13), one obtains the following conditions for the strain-functions (9) :

$$ (\frac{\partial\,{}^{t}\hat{\underset{\sim}{F}}^T}{\partial\,{}^{t}\underset{\sim}{F}_e})^{-1} = \underset{\approx}{1}.\,{}^{t}\underset{\sim}{F}_e^T.\,{}^{t}\underset{\sim}{F}^{-T} = (\frac{\partial\,{}^{t}\hat{\underset{\sim}{\Gamma}}^T}{\partial\,{}^{t}\underset{\sim}{\Gamma}_e})^{-1}, \underset{\approx}{A}..\underset{\approx}{1} = \underset{\approx}{1}..\underset{\approx}{A} = \underset{\approx}{A}. \qquad (14) $$

The inverse of $\underset{\approx}{1}.\,{}^{t}\underset{\sim}{F}_e^T.\,{}^{t}\underset{\sim}{F}^{-T}$ is ${}^{t}\underset{\sim}{F}^T.\,{}^{t}\underset{\sim}{F}_e^{-T}.\underset{\approx}{1}$. Thus,

$$ \frac{\partial\,{}^{t}\hat{\underset{\sim}{F}}^T}{\partial\,{}^{t}\underset{\sim}{F}_e} = \underset{\sim}{P}^T.\underset{\approx}{1}, \quad \underset{\sim}{P}^T := {}^{t}\underset{\sim}{F}^T\,{}^{t}\underset{\sim}{F}_e^{-T} \quad \Leftrightarrow \quad {}^{t}\underset{\sim}{F}^T = \underset{\sim}{P}^T\,{}^{t}\underset{\sim}{F}_e^T. \qquad (15) $$

Generally, the partial differential of ${}^{t}\hat{\underset{\sim}{F}}^T$ with respect to ${}^{t}\underset{\sim}{F}_e$ is by differentiation of (15)c

$$ \frac{\partial\,{}^{t}\hat{\underset{\sim}{F}}^T}{\partial\,{}^{t}\underset{\sim}{F}_e}..d\,{}^{t}\underset{\sim}{F}_e^T = \underset{\sim}{P}^T.\underset{\approx}{1}..d\,{}^{t}\underset{\sim}{F}_e^T + \underset{\approx}{1}_T..({}^{t}\underset{\sim}{F}_e.\frac{\partial\hat{\underset{\sim}{P}}}{\partial\,{}^{t}\underset{\sim}{F}_e})..d\,{}^{t}\underset{\sim}{F}_e^T, \quad \underset{\approx}{A}..\underset{\approx}{1}_T = \underset{\approx}{1}_T..\underset{\approx}{A} = \underset{\approx}{A}^T. \qquad (16) $$

But the first term of that is, according to eq. (15)a, the partial derivative of $\hat{\underset{\sim}{F}}^T$ itself! Therefore the partial derivative of $\hat{\underset{\sim}{P}}$ with respect to ${}^{t}\underset{\sim}{F}_e$ must vanish and hence $\hat{\underset{\sim}{P}}$ cannot depend on ${}^{t}\underset{\sim}{F}_e$. From the representation (15)c and the condition (10)e, one gets

$$ {}^{t}\hat{\underset{\sim}{F}}({}^{t}\underset{\sim}{F}_e=\underset{\approx}{1},\ {}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)\equiv\hat{\underset{\sim}{P}}({}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)\equiv {}^{t}\underset{\sim}{F}_p \qquad (17) $$

and thus a decomposition of the strain ${}^{t}\underset{\sim}{F}$:

$$ {}^{t}\underset{\sim}{F} = {}^{t}\underset{\sim}{F}_e\,{}^{t}\underset{\sim}{F}_p. \qquad (18) $$

Comparing that with Mandel's split $\underset{\sim}{F} = \underset{\sim}{E}\underset{\sim}{P} = \underset{\sim}{R}\,{}^{t}\underset{\sim}{F}$ [3], one sees a generalized polar decomposition of $\underset{\sim}{E}$: $\underset{\sim}{E} = \underset{\sim}{R}\,{}^{t}\underset{\sim}{F}_e$. According to the condition (14)b, the same representation as (15)a is valid for the partial derivative of ${}^{t}\hat{\underset{\sim}{\Gamma}}^T$ with respect to ${}^{t}\underset{\sim}{\Gamma}_e$, but now with the identification (17)b :

$$ \frac{\partial\,{}^{t}\hat{\underset{\sim}{\Gamma}}^T}{\partial\,{}^{t}\underset{\sim}{\Gamma}_e} = {}^{t}\underset{\sim}{F}_p^T.\underset{\approx}{1} \Leftrightarrow \frac{\partial\,{}^{t}\hat{\underset{\sim}{\Gamma}}}{\partial\,{}^{t}\underset{\sim}{\Gamma}_e}..d\,{}^{t}\underset{\sim}{\Gamma}_e^T = d\,{}^{t}\underset{\sim}{\Gamma}_e\,{}^{t}\underset{\sim}{F}_p. \qquad (19) $$

Integration of this differential gives ${}^{t}\hat{\underset{\sim}{\Gamma}}({}^{t}\underset{\sim}{\Gamma}_e,\ {}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p) = {}^{t}\underset{\sim}{\Gamma}_e\,{}^{t}\underset{\sim}{F}_p + \hat{\underset{\sim}{P}}_2({}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)$ and with the condition (10)f, one gets ${}^{t}\hat{\underset{\sim}{\Gamma}}({}^{t}\underset{\sim}{\Gamma}_e=\underset{\sim}{0},\ {}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)\equiv\hat{\underset{\sim}{P}}_2({}^{t}\underset{\sim}{F}_p,\ {}^{t}\underset{\sim}{\Gamma}_p)\equiv {}^{t}\underset{\sim}{\Gamma}_p$, and *a decomposition of the wryness tensor* is implied :

$$ {}^{t}\underset{\sim}{\Gamma} = {}^{t}\underset{\sim}{\Gamma}_e\,{}^{t}\underset{\sim}{F}_p + {}^{t}\underset{\sim}{\Gamma}_p. \qquad (20) $$

The decompositions (18) and (20) have been assumed in [18]. Then the elastic constitutive equations (13) follow necessarily. These decompositions were completely independently developed in [17] as shown above.

The form of the function (20) is similar to that used in [11] as symmetry transformation of a Cosserat fluid. This is not so surprisingly, because the interpretation of a symmetry transformation as plastic deformation has been already pointed out in [19] for classical continua. A difference is that at the Cosserat continuum a rigid rotation as a symmetry transformation (defining solids) is not considered as plastic [17] but this has been suggested in [19].

The most simple decomposition of the wryness tensor is the purely additive decomposition ${}^{t}\underset{\sim}{\Gamma} = {}^{t}\underset{\sim}{K}_e + {}^{t}\underset{\sim}{\Gamma}_p$ in [20]. This fits also in the general framework (9). If (20) is not true, then the hyperelastic relations for the stresses do not have the form (13) at large plastic strain as in the pure hyperelastic case. The reason is that, at the purely additive decomposition, the same strain-energy of elasticity is stored at the same wryness of a unit length of the initial configuration : $\hat{\psi}_e({}^{t}\underset{\sim}{F}_e,\ {}^{t}\underset{\sim}{K}_e)$. This means a constitutive behaviour where the wryness-elasticity with respect to the intermediate configuration, i.e. a strain-energy function of ${}^{t}\underset{\sim}{\Gamma}_e$ of (20), $\hat{\psi}_e({}^{t}\underset{\sim}{F}_e,\ {}^{t}\underset{\sim}{K}_e = {}^{t}\underset{\sim}{\Gamma}_e\,{}^{t}\underset{\sim}{F}_p) =: \hat{\psi}_{\hat{\underset{\sim}{F}}^p}({}^{t}\underset{\sim}{F}_e,\ {}^{t}\underset{\sim}{\Gamma}_e)$ changes due to plastic straining (that is the ${}^{t}\underset{\sim}{F}_p$-dependence of $\hat{\psi}_{\hat{\underset{\sim}{F}}^p}$). But this seems to be questionable for metals according to the lattice concept (see section 4.2).

4. APPLICATION TO CRYSTAL PLASTICITY

The previous developments are now readily applied to the case of single crystal plasticity.

4.1. Dislocation densities

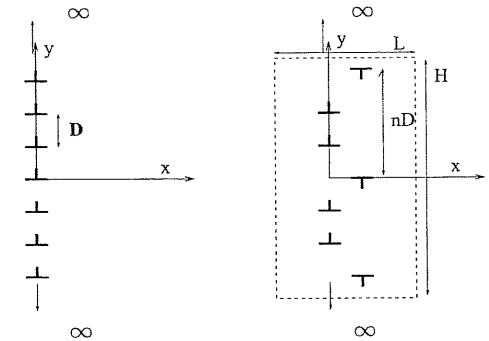

Figure 1 : (a) ideal tilt boundary (b) alternate tilt boundary.

The predictive capabilities of a constitutive model of the plastic behavior of single crystals strongly depends on the accuracy of the description of the dislocation population inside the volume element of continuum mechanics. A complete description of this distribution would require an infinite set of correlation functions as Kröner pointed out [21]. Only two of them are actually used in practise, and in two different contexts. 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 appropriate description of dislocation distribution in the continuum theory of dislocations is given by Nye's dislocation density tensor [22] defined by : $\underline{b} = \int_S \underset{\sim}{\alpha}\,\underline{n}\,dS$, with $\underset{\sim}{\alpha} = -\mathrm{curl}\,({}^{t}\underset{\sim}{F}_e^{-1}\,\underset{\sim}{R}^T)$ where $\underline{b}$ is the resulting true Burgers vector for a surface S bounded by a closed line in the current configuration, and where the decomposition (18) has been used. In other terms, the dislocation density tensor is directly related to the densities ρ_G of so-called geometrically necessary dislocations [23]. On the other hand, classical crystal plasticity

theory which aims at describing the hardening behaviour of crystals, resorts to internal variables connected with the densities ρ_S of statistically stored dislocations [23].

The following example will show that the two quantities ρ_S and ρ_G are independent descriptions of the complex distribution of dislocations in a volume element. Consider a volume element of size $L \times H \times 1$ containing an idealized distribution of dislocations that we call an alternate tilt boundary (figure 1b). The densities ρ_G and ρ_S are in this case : $\rho_S = 1/DL$, $\rho_G = n - 2/nDL$. It can be seen that ρ_S, being the total length of dislocation lines in the element, is not sensitive to the signs of the burgers vectors so that it does not depend on n. On the contrary, ρ_G goes from 0 ($n = 2$) and tends to ρ_S for increasing n (ideal tilt boundary, figure 1a).

A distribution of tilt boundaries can be used to represent lattice curvature. The lattice misorientation associated with an alternate tilt boundary increases for increasing n and vanishes for $n = 2$. It is thought that the hardening behaviours induced by each type of dislocation densities are different. Furthermore the resistance to lattice curvature formation can be accounted for in a continuous manner by introducing couple stresses [24]. This motivates the following developments. Since it corresponds to a gradient of lattice rotation, the density of geometrically necessary dislocations becomes important in the presence of strongly non-homogeneous deformation. This may be the case at a microscopic level at the beginning of plastic flow, in particular in the presence of second phase, and, at a macroscopic scale, when deformation localizes (see section 5).

A similar reckoning can be done in the case of twist and alternate twist boundaries made of regular populations of screw dislocations, accounting for lattice torsion.

4.2. Single crystal kinematics

The relative independence of the quantities ρ_S and ρ_G can be translated in kinematical terms : The rotation of lattice directions due to plastic deformation is not directly related to the rotation of material lines. This explains why lattice rotation $\underset{\sim}{\mathbf{R}}$ and mean displacement $\underline{\mathbf{u}}$ are regarded as independent degrees of freedom at material point $\underline{\mathbf{x}}$ in the sequel. In classical crystal plasticity, lattice rotation merely has the status of a hidden variable. The necessity of the construction of a Cosserat theory for single crystals is suggested by Mandel as a natural extension of crystal plasticity in [3]. The first proposal for a multiplicative decomposition of the deformation gradient $\underset{\sim}{\mathbf{F}}$ into an elastic and a plastic part probably goes back to the late fifties [25] and the argument is based on the introduction of a local intermediate released configuration. The cutting and releasing operations on a material element lead to the definition of the equivalent Burgers vector and give the remaining plastic deformation $\underset{\sim}{\mathbf{F}}_p$. However there was an indeterminacy in choosing the orientation of the released material element. Mandel [3] solved that problem by choosing the so-called isoclinic released configuration which has the orientation of a fixed reference lattice.

If lattice curvature is considered, the decomposition (20) derived in section 3 enables us to define a local intermediate released configuration for the couple stresses, which coincides with the released configuration for the force stresses. In this state of the material element, couple and force stresses vanish and only permanent deformation and curvature are observable. The decomposition (20) can be written : $\underset{\sim}{\Gamma} = \underset{\sim}{\mathbf{R}}\, {}^\sharp\underset{\sim}{\Gamma} = \underset{\sim}{\Gamma}_e \underset{\sim}{\mathbf{F}}_p + \underset{\sim}{\Gamma}_p$ with $\underset{\sim}{\Gamma}_e = \underset{\sim}{\mathbf{R}}\, {}^\sharp\underset{\sim}{\Gamma}_e$, $\underset{\sim}{\Gamma}_p = \underset{\sim}{\mathbf{R}}\, {}^\sharp\underset{\sim}{\Gamma}_p$ and $\underset{\sim}{\mathbf{F}}_p = {}^\sharp\underset{\sim}{\mathbf{F}}_p$. The different linear applications are represented in figure 2. Consider a material segment $d\underline{\mathbf{x}}$ on the current configuration, it is related to the material segment $d\underline{\mathbf{X}}$ on the reference configuration by $d\underline{\mathbf{x}} = \underset{\sim}{\mathbf{F}}\, d\underline{\mathbf{X}} = \underset{\sim}{\mathbf{F}}_e d\underline{\mathbf{x}}^i$ with $d\underline{\mathbf{x}}^i = \underset{\sim}{\mathbf{F}}_p\, d\underline{\mathbf{X}}$. Similarily, the variation of micro-rotation along a material segment is given by $-\frac{1}{2}\underset{\sim}{\epsilon}(d\underset{\sim}{\mathbf{R}}\, \underset{\sim}{\mathbf{R}}^T) = \underset{\sim}{\Gamma}\, d\underline{\mathbf{X}} = \underset{\sim}{\Gamma}_e d\underline{\mathbf{x}}^i + \underset{\sim}{\Gamma}_p d\underline{\mathbf{X}}$. The elastic contribution to deformation and curvature can therefore be considered simultaneously with respect to the material segment $d\underline{\mathbf{x}}^i$ on the intermediate configuration. Note that this definition of the intermediate released configuration would not have been possible with the purely additive decomposition proposed in [20].

The plastic deformation rate is then due to the contributions of N slip systems. Similarily, plastic lattice torsion and curvature develop according to special crystallographic directions. Thus

$$ {}^\sharp\dot{\underset{\sim}{\mathbf{F}}}_p\, {}^\sharp\underset{\sim}{\mathbf{F}}_p^{-1} = \sum_{s=1}^{N} \dot{\gamma}^s\, {}^\sharp\underset{\sim}{\mathbf{P}}^s \quad \text{and} \quad {}^\sharp\dot{\underset{\sim}{\Gamma}}_p\, {}^\sharp\underset{\sim}{\mathbf{F}}_p^{-1} = \sum_{s=1}^{N} \frac{\dot{\theta}^s}{l}\, {}^\sharp\underset{\sim}{\mathbf{Q}}^s \qquad (21) $$

with ${}^\sharp\underset{\sim}{\mathbf{P}}^s = {}^\sharp\underline{\mathbf{m}}^s \otimes {}^\sharp\underline{\mathbf{z}}^s$, dyadic product of the slip direction vector and the normal to the glide plane. If lattice torsion is not considered, ${}^\sharp\underset{\sim}{\mathbf{Q}}^s = {}^\sharp\underline{\xi}^s \otimes {}^\sharp\underline{\mathbf{m}}^s$, where ${}^\sharp\underline{\xi}^s = {}^\sharp\underline{\mathbf{z}}^s \times {}^\sharp\underline{\mathbf{m}}^s$ is the dislocation line vector of edge dislocations.

5. FINITE ELEMENT SIMULATION OF COSSERAT CRYSTALS

Some localization modes in single crystals are associated with strong lattice rotation gradients so that their simulation seems to be a good test of the physical relevance of a generalized model.

A viscoplastic formulation of crystal plasticity is retained :

$$ \dot{\gamma}^s = \left(\frac{\mathrm{Max}(0, |\ \tau^s\ | - r^s)}{k}\right)^n \mathrm{sign}\ (\tau^s), \text{ and } \dot{\theta}^s = \left(\frac{\mathrm{Max}(0, |\ {}^\sharp\underset{\sim}{\boldsymbol{\mu}} :\ {}^\sharp\underset{\sim}{\mathbf{Q}}^s\ | - l r_c)}{l k_c}\right)^{n_c} \mathrm{sign}\ ({}^\sharp\underset{\sim}{\boldsymbol{\mu}} :\ {}^\sharp\underset{\sim}{\mathbf{Q}}^s) \qquad (22) $$

where $\tau^s = {}^\sharp\underset{\sim}{\boldsymbol{\sigma}} :\ {}^\sharp\underset{\sim}{\mathbf{P}}^s$, $\dot{v}^s = |\ \dot{\gamma}^s\ |$ and $r^s = r_0 + \sum_{r=1}^{N} H^{sr}(1 - e^{-bv^r}) + H'\theta^r$ is the hardening law. In this work, r_c is constant. More general constitutive equations with their thermodynamical formulation can be found in [14]. The simplified version presented here will be used in the next simulation and involve a coupling term H' between plastic deformation and curvature. The internal variables v^s (cumulative slip) and θ^s (non-cumulative lattice curvature) can be regarded as an estimation of the densities ρ_S and ρ_G respectively.

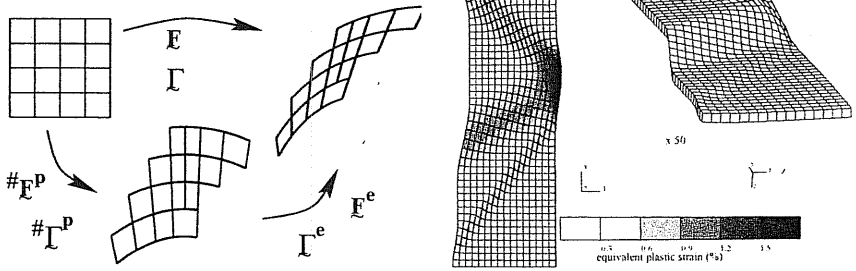

Figure 2 : Kinematics of the deformation and curvature of single crystals.

Figure 3 : Strain localisation in a single crystal (symmetric double slip) : (a) contour of equivalent plastic strain, (b) deformed state.

The two possible strain localization modes in single crystals undergoing single slip are called slip and kink bands [26]. The localization planes respectively are the slip plane and the plane normal to the glide direction $\underline{\mathbf{m}}$ (kink plane). In the case of initially symmetric double slip, symmetric and symmetry breaking modes exist depending on the form of the hardening matrix H^{sr} [26]. An example of symmetry-breaking mode is now given. A f.c.c. single crystal plate oriented for double slip in tension is considered. Its width is $1L$. Strain softening is introduced in the constitutive behaviour so that a material defect (a slightly lower initial critical resolved shear stress in one element) will induce strain localization. The hardening matrix H^{sr} has been taken diagonal in this work. The Cosserat single crystal model has been implemented in a finite element program. The additional Cosserat parameters are : $H' = 600\,\mathrm{MPa}, r_c^0 = 0.0005\,\mathrm{MPa}, k_c = 0.01\mathrm{MPa\,s}^{1/n_c}, n_c = 1, l = 1L$. The Cosserat elasticity parameters are taken so small that classical elasticity is unaffected.

If classical plasticity is used, a symmetry-breaking bifurcation mode is obtained as shown on figure 3. Three bands form in which single slip only occur : 2 slip bands and one kink band. As shown on figure 5a, the kink band is associated with strong lattice curvature. In constrast, the simulation of the same problem using Cosserat crystal plasticity leads to two slip bands only (figure 4a). The kink band has been precluded because it induces intense lattice curvature associated with additional

hardening due to the coupling term. These features are more relevant from the physical standpoint since kink bands are seldom observed in f.c.c. crystal except after large overall straining which was not the case in the simulation. The decisive difference between slip and kink bands within a Cosserat framework can also be derived from a bifurcation analysis in Cosserat crystal plasticity as in [26].

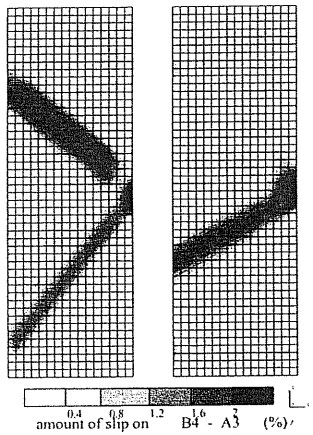

Figure 4 : Contours of amounts of slip for each slip system.

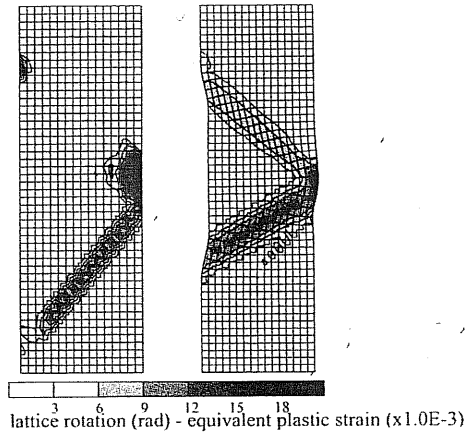

Figure 5 : Lattice rotation in a kink band (left, classical case); strain localization in a Cosserat crystal (right).

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A continuum mechanical gradient theory with applications to fluid mechanics

G. Silber*,**, R. Trostel**, M. Alizadeh* and G. Benderoth*

** Fachhochschule Frankfurt am Main, Labor für Materialwissenschaften (LabMat), Fachbereich Feinwerktechnik, Nibelungenplatz 1, 60318 Frankfurt am Main, Germany*
*** Technische Universität Berlin, Institut für Mechanik, Fachbereich Verkehrswesen und Angewandte Mechanik, Stresse des 17. Juni, 10623 Berlin, Germany*

Abstract. A gradient theory of grade two based on an axiomatic conception of a nonlocal continuum theory for materials of grade n is presentated. The total stress tensor of rank two in the equation of linear momentum contains two higher stress tensors of rank two and three. In the case of isotropic materials both the tensor of rank two and three are tensor-valued functions of the second order strain rate tensor and its first gradient so that the equation of motion is of order four. The necessary boundary conditions for real boundaries are generated by using so-called porosity tensors. This theory is applied to two experiments. To a velocity profile of a turbulent COUETTE flow of water and a POISEUILLE flow of a blood like suspension. On the basis of these experimental data the material and porosity coefficients are identified by numerical algorithms like evolution strategies.

1 INTRODUCTION

To describe the material behaviour of fluids and solids by a continuum mechanical theory a set of field equations containing mass, linear and angular momentum and a particular constitutive equation is needed. If the microstructure of the material is mechanically significant and the theory of simple materials cannot solve the problem, a more sensitive continuum theorie such as nonlocal, micropolar, multipolar and gradient theories [4, 5, 6, 13, 20, 21] with higher kinematic status will be applied more successfully. In this paper a gradient theory of grade two is used. This theory is based on an axiomatic conception of a nonlocal continuum theory for materials of grade n by Trostel [22, 23] with applications to turbulent flow of Newtonian fluids and laminar flow of non-Newtonian fluids (especially biosuspensions). A comprehensive review of existing theories of microcontinuum fluid mechanics with various applications has been presented by Ariman, Turk and Sylvester [3]. But most of the papers cited there don't do a proper identification of the material coefficients for the used mechanical models. In this paper some ideas for identification of material parameters based on experimental data are given.

2 METHODS

The used continuum coincides with the description of motion in an ordinary continuum characterized kinematically only by a velocity field. But the higher sensitiveness of the body is considered by modification of the principle of local neighborhood, that means that not only the first but higher velocity gradients are admitted in the kinematical description. Hence, there are stress and dual strain rate tensors not only of second but higher ranks depending on the grade of the used model.

The conception of Trostel [22] is based on the first law of thermodynamics and special structural forms of kinetic and internal energy as well as mechanical and nonmechanical power. Using the requirements of Rational Mechanics especially determinism, objectivity and modified local neighborhood the field equations of linear and angular momentum as well as the structural forms for the set of stress tensors are developed. For a material of grade n there are n higher stress tensors from rank two up to rank n + 1 which are de-