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STRAIN MEASURES, INTEGRABILITY CONDITION AND FRAME INDIFFERENCE IN THE THEORY OF ORIENTED MEDIA*

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Abstract-This paper is concerned with the appropriate choice of state variables within the continuum model or oriented media. It is shown that residual deformation, strain and wryness can be considered as such quantities. The compatibility conditions for them are derived, which make the inverse problem of determining the displacement and director triad fields well-posed. The principle offrame indifference justifies the use ofthese quantities as state variables in the free energy density. Governing and constitutive equations are studied in detail. A comparison with the continuum model of crystals with continuously distributed dislocations is provided. $@$ 1997 Elsevier Science Ltd.

1. INTRODUCTION

In various problems of materials science the influence of the microstructure on the mechanical behaviour can be of major importance. Such problems are, among others, the localization of shear bands in single crystals, the evolution of micro- and macrocracks and the martensite phase transition. The account of microstructure can be made by introducing a triad of vectors (directors) attached to each point of the continuum [Cosserat and Cosserat (1907); Toupin (1964); Truesdell and Noll (1965)]. It is essential then to extend the concept of motion of such materials involving also the transformation law of the triads. The latter, complementing the displacement field, should be regarded as additional degrees-of-freedom of the theory with microstructure.

The next logical step in developing the kinematics of oriented continua is associated with an appropriate choice of strain measures. The latter depends on the definition of the rigid-body motions of materials in such a manner, that the once chosen strain measures should characterize fully the displacement and director distortion fields up to a rigid-body motion. Eringen and Kafadar (1977) presented a list of strain measures consisting of the residual distortion, director deformation and wryness. They also derived the compatibility conditions for them.

A system of static equations (of dynamic equations in general) for the oriented continua can be derived by postulating the principle of virtual work (or the action principle). This leads to the well-established balance of momentum and director momentum [Toupin (1964); Capriz and Podio-Guidugli (1976); Capriz (1989)]. For oriented continua, whose mechanical response is determined by a single function called the free energy density, constitutive equations for the stresses, director stresses and couple-stresses can be established. This completes the construction of the model.

In this paper, we derive formulae expressing the displacement and director distortion fields in terms of the residual distortion, director deformation and torsion fields, provided the compatibility conditions are fulfilled. These formulae are similar to those derived recently by Le and Stumpf (1996a) in the continuum theory of dislocations. They clearly show that the displacement and director deformation fields are determined from the residual distortion, director deformation and torsion fields uniquely up to a rigid-body motion. Using the principle of frame indifference, we justify the use of the residual distortion, director deformation and wryness as state variables in the constitutive equations (or in the free energy density, if it exists). Further consequences of this result for the constitutive

* Dedicated to Professor Erwin Stein on the occasion of his 65th birthday.

equations will be shown. By identifying the directors with the lattice vectors and the director distortion with the elastic distortion, governing and constitutive equations for crystals and polycrystals can be derived. For crystals (or polycrystals) containing continuously distributed dislocations Kroner (1992) and Le and Stumpf (1994) require the free energy density per unit volume of the reference crystal to depend only on the elastic deformation and on the torsion (it satisfies then the principle of frame indifference as well as the principle ofinitial scaling indifference). In this special case, and provided the microtraction specified on the boundary is zero, the governing and constitutive equations for oriented continua are shown to be equivalent to those derived in the recently proposed micromodels of finite elastoplasticity [Stumpf and Le (1993); Le and Stumpf (1994, 1996a,b,c); Naghdi and Srinivasa (1993, 1994)], if the dissipation there is not taken into account. Despite this fact, the equations proposed in Le and Stumpf (1994, 1996a,b,c) are formulated in clear and physically tractable stress measures so that it is more convenient to use them instead of those in Toupin (1964), Capriz and Podio-Guidugli (1976) and Capriz (1989).

2. STRAIN MEASURES

Let us consider a body \mathcal{B} , whose points X, Y, ..., $\in \mathcal{B}$ can be identified with their position vectors **X**, **Y**, ..., $\in \mathscr{E}$ in a fixed reference configuration, where \mathscr{E} is the threedimensional Euclidean space. A motion of this body can be described by means of smooth invertible functions $\phi(\mathbf{X}, t)$

$$
\mathbf{x} = \boldsymbol{\phi}(\mathbf{X}, t) = \mathbf{X} + \mathbf{u}(\mathbf{X}, t),
$$
 (1)

with $\mathbf{x} \in \mathscr{E}$ the position vector in the current configuration and $\mathbf{u}(\mathbf{X}, t)$ the displacement field. Introducing basis vectors G_A and g_a and their duals G^A and g^a at X and x, respectively, one can define the deformation gradient F and its determinant J by

$$
\mathbf{F} = \partial \boldsymbol{\phi} / \partial \mathbf{X} = F_{\mathbf{A}}^{\mathbf{a}} \mathbf{g}_{\mathbf{a}} \otimes \mathbf{G}^{\mathbf{A}}, \quad J = \text{det} \mathbf{F}.
$$
 (2)

We further stipulate that $J > 0$. Throughout the paper, summation convention for repeated indices is employed. With the metric tensor $g = g_{ab}g^a \otimes g^b$ of the Euclidean space, also referred to as the isomorphism from the translation space \mathcal{V}^* to its dual space \mathcal{V} , the Cauchy-Green deformation tensor C is defined by

$$
\mathbf{C} = \mathbf{F}^{\mathrm{T}} \mathbf{g} \mathbf{F} = C_{AB} \mathbf{G}^{A} \otimes \mathbf{G}^{B}, \quad C_{AB} = F_{A}^{a} g_{ab} F_{B}^{b}.
$$

This tensor C remains unchanged under a superposed rigid-body motion. Therefore, in classical continuum mechanics, it is rightly referred to as state variable in the constitutive equations.

By an oriented continuum we will understand now a body $\mathscr B$ endowed at each point with a triad of deformable, linearly independent vectors, or directors, in Toupin's terminologyt [see Toupin (1964); Truesdell and Noll (1965)]. We denote the triad of directors at **X** by $\mathscr{D}_{\alpha} \in \mathscr{V}$, $\alpha = 1, 2, 3.1$ The motion of such a body can be described by eqn (1) and the two-point tensor

$$
\mathbf{D} = d_{\alpha} \otimes \mathscr{D}^{\alpha} = D_{\mathbf{A}}^{\alpha} \mathbf{g}_{\mathbf{a}} \otimes \mathbf{G}^{\mathbf{A}},\tag{3}
$$

which maps the triad \mathscr{D}^{α} at **X** into the triad d_{α} , $\alpha = 1, 2, 3$ at **x**

t In the modern literature this continuum is also called continuum with affine microstructure or micromorphic continuum [see Eringen and Kadafar (1977); Capriz and Podio-Guidugli (1976); Capriz (1989)].

t Greek indices are used to numerate the directors.

$$
d_{\alpha} = \mathbf{D}\mathcal{D}_{\alpha}.\tag{4}
$$

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The field D will be called the director distortion field. Here the reciprocal director triads \mathscr{D}^{α} , d^{α} (one-forms) are defined through the relations

$$
\mathscr{D}^{\alpha} \cdot \mathscr{D}_{\beta} = d^{\alpha} \cdot d_{\beta} = \delta^{\alpha}_{\beta},
$$

where the symbol δ_{θ}^s stands for the Kronecker delta and the dot denotes the scalar product of dual tensors. The determinant of **D** is supposed to be positive. We regard $D(X, t)$ as an additional unknown field, which, together with $\phi(X, t)$, characterizes fully the motion of the oriented continuum.

The triad \mathscr{D}_{α} can be expressed in terms of G_A through the following relation

$$
\mathscr{D}_{\alpha} = Y_{\alpha}^{\mathbf{A}} \mathbf{G}_{\mathbf{A}},\tag{5}
$$

where the matrix Y_{α}^{A} in general is not derivable from any coordinate transformation. Using the anholonomic base \mathscr{D}_x , we can represent **D** in the form

$$
\mathbf{D} = D_A^{\mathsf{a}} Y_\alpha^{\mathsf{A}} \mathbf{g}_{\mathsf{a}} \otimes \mathscr{D}^{\alpha} = \bar{D}_{\mathsf{a}}^{\mathsf{a}} \mathbf{g}_{\mathsf{a}} \otimes \mathscr{D}^{\gamma} \tag{6}
$$

Representations of this type have been used frequently in finite elastoplasticity with microstructure [Le and Stumpf (1994)].

Let us seek the set of kinematic variables, which plays the same role in the theory of oriented continuum as C in classical continuum mechanics. We introduce the following field

$$
\mathbf{H} = \mathbf{D}^{-1} \mathbf{F} = H_B^A \mathbf{G}_A \otimes \mathbf{G}^B, \quad H_B^A = (\mathbf{D}^{-1})_a^A F_B^a \tag{7}
$$

which is called residual distortion. When the director distortion D and the deformation gradient F are equal, that means the element and the directors are deformed together, then $H = 1$. Thus, H measures the difference between the compatible deformation gradient F and the (in general) incompatible director distortion D. For crystals and polycrystals it will be shown, in Section 6, that D can be identified with the elastic distortion and H corresponds then to the plastic distortion. Referring to the anholonomic base \mathscr{D}_{α} we have

$$
\mathbf{H} = \bar{H}_{\mathbf{A}}^{\alpha} \mathscr{D}_{\alpha} \otimes \mathbf{G}^{\mathbf{A}}, \quad \bar{H}_{\mathbf{A}}^{\alpha} = (\mathbf{D}^{-1})_{a}^{\alpha} F_{\mathbf{A}}^{\alpha}.
$$
 (8)

Next, we introduce the symmetric tensor field

$$
\mathbf{C}^{\mathsf{I}} = \mathbf{D}^{\mathrm{T}} \mathbf{g} \mathbf{D} = C_{AB}^{\mathsf{I}} \mathbf{G}^{\mathsf{A}} \otimes \mathbf{G}^{\mathsf{B}}, \quad C_{AB}^{\mathsf{I}} = D_{A}^{a} g_{ab} D_{B}^{b}, \tag{9}
$$

which is called director deformation. With C_{AB}^1 one can measure lengths (and angles) of the deformed directors through the undeformed ones. Indeed, let \mathscr{D}_1 and \mathscr{D}_2 be two directors given by

$$
\mathscr{D}_1 = Y_1^{\mathbf{A}} \mathbf{G}_{\mathbf{A}}, \quad \mathscr{D}_2 = Y_2^{\mathbf{B}} \mathbf{G}_{\mathbf{B}}.
$$

Then from eqns (4) and (9) we have

 $\tilde{\mathbf{r}}_{\text{tot}}$

$$
\mathbf{g}(d_1, d_2) = g_{ab} D_A^a D_B^b Y_1^A Y_2^B = C_{AB}^l Y_1^A Y_2^B.
$$

The components of C' with respect to the anholonomic base \mathscr{D}_α give the lengths and angles of the corresponding deformed directors directly. For crystals and polycrystals $C¹$ will be identified with the elastic deformation field.

Finally, we introduce the gradient of D with respect to the reference configuration

$$
GradD = D_{C,B}^{a} \mathbf{g}_{a} \otimes \mathbf{G}^{B} \otimes \mathbf{G}^{C},
$$
\n(10)

wherein the component representation we use for simplicity cartesian coordinates so that the comma preceding indices denotes the partial derivatives with respect to the corresponding coordinates. Pulling back one leg of this tensor with D to the reference configuration, we obtain the third rank tensor field

$$
\Gamma = (\mathbf{D}^{-1})_a^A D_{C,B}^a \mathbf{G}_A \otimes \mathbf{G}^B \otimes \mathbf{G}^C, \tag{11}
$$

which is called wryness. Its components $\Gamma_{BC}^A = (\mathbf{D}^{-1})^A_a D_{CB}^a$ can be interpreted as the Christoffel symbols of the connection ∇ induced by D as follows

$$
\nabla_{\mathbf{W}_1} \mathbf{W}_2 = (W_{2,B}^{\mathbf{A}} W_1^{\mathbf{B}} + \Gamma_{BC}^{\mathbf{A}} W_2^{\mathbf{C}} W_1^{\mathbf{B}}) \mathbf{G}_{\mathbf{A}},
$$
(12)

with $W_1 = W_1^B G_B$, $W_2 = W_2^C G_C$ two arbitrary vectors. It is easy to prove that (12) qualifies itself as the connection. The distinguished feature of this connection is that $\nabla_{\mathbf{W}_1} \mathbf{V} = 0$ for every vector field V , which is the pull-back of a constant vector \bf{v} by \bf{D} . The skew-symmetric part of Γ

$$
\mathbf{T}^1 = (\mathbf{\Gamma})_{\text{skw}} = (\mathbf{D}^{-1})^{\text{A}}_{\text{a}} (D^{\text{a}}_{\text{C,B}} - D^{\text{a}}_{\text{B,C}}) \mathbf{G}_{\text{A}} \otimes \mathbf{G}^{\text{B}} \otimes \mathbf{G}^{\text{C}} \tag{13}
$$

forms the tensor field called torsion of the connection ∇ . For crystals and polycrystals we shall see that Γ is closely related to the dislocation density.

Since $C¹$ and Γ are derivable from the tensor field **D**, they should satisfy some compatibility conditions. Using differential geometry one can prove that the following compatibility condition

$$
\mathbf{R} = 0 \tag{14}
$$

has to be satisfied, with the fourth rank curvature tensor R given by [see, e.g. Sternberg (1983)]

$$
R_{\text{BCD}}^{\text{A}} = \Gamma_{\text{CE}}^{\text{A}} \Gamma_{\text{DB}}^{\text{E}} - \Gamma_{\text{DE}}^{\text{A}} \Gamma_{\text{CB}}^{\text{E}} + \Gamma_{\text{DB,C}}^{\text{A}} - \Gamma_{\text{CB,D}}^{\text{A}}, \tag{15}
$$

which means that the curvature of the connection ∇ vanishes [see the proof in Noll (1967)].

Following Noll (1967), one can also introduce the third rank tensor field K with the components

$$
K_{\text{BC}}^{\text{A}} = \Gamma_{\text{BC}}^{\text{A}} - \begin{Bmatrix} \text{A} \\ \text{BC} \end{Bmatrix},\tag{16}
$$

with ${A \choose BC}$ the Christoffel symbol of the Riemannian connection induced by the strain tensor field \mathbb{C}^1 . We call **K** the contortion tensor field. Torsion and contortion determine each other in the following sense [Noll (1967)]

$$
K_{BC}^{A} = \frac{1}{2} [(\mathbf{T}^{l})_{BC}^{A} - C_{BD}^{l}(\mathbf{T}^{l})_{CE}^{D} (\mathbf{C}^{l-1})^{EA} - C_{CD}^{l}(\mathbf{T}^{l})_{BE}^{D} (\mathbf{C}^{l-1})^{EA}].
$$
 (17)

Let us find out the compatibility condition for H. Since F is the deformation gradient, the following equations hold true

$$
F_{\mathbf{A},\mathbf{B}}^{\mathbf{a}} - F_{\mathbf{B},\mathbf{A}}^{\mathbf{a}} = 0. \tag{18}
$$

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Substituting $\mathbf{F} = \mathbf{D}\mathbf{H}$ from eqn (7) into (18) and contracting the obtained equation with \mathbf{D}^{-1} we get

$$
\Gamma_{\rm CD}^{\rm A} H_{\rm B}^{\rm D} - \Gamma_{\rm BD}^{\rm A} H_{\rm C}^{\rm D} + H_{\rm B,C}^{\rm A} - H_{\rm C,B}^{\rm A} = 0. \tag{19}
$$

Equation (19) can also be considered, together with eqns (14) and (17), as the compatibility conditions for H, C^1 and Γ [cf. Eringen and Kafadar (1977)].

3. INTEGRABILITY CONDITION

In classical continuum mechanics it is well known, that the knowledge ofthe Cauchy-Green deformation tensor field C is sufficient to determine the deformation gradient F and subsequently the displacement field u uniquely up to a rigid body motion, provided C satisfies the Riemann compatibility conditions. Now let us consider the inverse problem of determining **u** and **D** from the given fields H, C', T' , provided the compatibility conditions (14), (17) and (19) are fulfilled. There are nine independent components of the residual distortion tensor field H , six of the symmetric deformation tensor field $C¹$, and nine of the torsion field $T¹$, from which 12 components of **u** and *D* should be determined. The similar problem in the nonlinear continuum theory of dislocations is considered in Le and Stumpf (1996a).

To solve this problem, let us first determine **D** from $C¹$ and $T¹$. The system of partial differential equations for **D** reads

$$
D_{\rm B,C}^{\rm a} = D_{\rm A}^{\rm a} \Gamma_{\rm CB}^{\rm A},\tag{20}
$$

where Γ_{BC}^{A} are the Christoffel symbols of the connection V. In this section we shall work out formulae explicitly in components. Note that the Γ_{BC}^{A} can also be expressed through C' and $T¹$ according to eqns (16) and (17), namely

$$
\Gamma_{BC}^{A} = \begin{Bmatrix} A \\ BC \end{Bmatrix} + K_{BC}^{A} = \frac{1}{2} C^{l-1} A^{D} [C_{BD,C}^{l} + C_{CD,B}^{l} - C_{BC,D}^{l}] + \frac{1}{2} [(T^{l})_{BC}^{A} - C_{BD}^{l} (T^{l})_{CE}^{D} (C^{l-1})^{EA} - C_{CD}^{l} (T^{l})_{BE}^{D} (C^{l-1})^{EA}].
$$
 (21)

Equation (20) can be considered as a system of partial differential equations for the nine components of D. The existence of the solution of (20) is ensured, if the following integrability conditions are fulfilled

$$
D_{\rm B,DC}^{\rm a} - D_{\rm B,CD}^{\rm a} = 0. \tag{22}
$$

Let us calculate the second derivative of D taking eqn (20) into account

$$
D_{\text{B,DC}}^{\text{a}} = D_{\text{A}}^{\text{a}} [\Gamma_{\text{CI}}^{\text{A}} \Gamma_{\text{DB}}^{\text{I}} + \Gamma_{\text{DB,C}}^{\text{A}}]. \tag{23}
$$

Substituting eqn (23) into the integrability conditions (22), we can rewrite them in the form

$$
D_{\rm A}^{\rm a} R_{\rm BCD}^{\rm A} = 0,\tag{24}
$$

with R_{BCD}^A the components of the curvature tensor (15). Thus eqn (24) is equivalent to eqn

Fig. 1. A motion of an oriented medium.

(14) and expresses nothing else, but the fact that the curvature of the connection ∇ has to vanish.

If the condition (14) is fulfilled, one can integrate eqn (20) to determine **D**. Let us fix some arbitrary point X_0 of the body. Let $c(s)$ be a curve connecting X_0 with another arbitrary point X such that $c(0) = X_0$ (Fig. 2). In the reference configuration this curve is described by the equation

$$
X^A = X^A(s), \quad X^A(0) = X_0^A. \tag{25}
$$

Multiplying both sides of eqn (20) by the tangent vector \dot{X}^c of the curve (the dot denotes here the derivative with respect to s) we get

$$
\frac{\mathrm{d}}{\mathrm{d}s}\mathbf{D} = \mathbf{D}\mathbf{P} \tag{26}
$$

with the tensor **P** having the components

$$
P_{\rm B}^{\rm A} = \Gamma_{\rm CB}^{\rm A} \dot{X}^{\rm C}.
$$
 (27)

Thus, the system of partial differential equations for D is transformed into the linear ordinary differential equation for **D** along the curve $c(s)$ with the tensor **P** as the given function of *s*. The solution of eqn (27) can be found in the form [see Gantmacher (1960)]

$$
\mathbf{D} = \mathbf{D}_0 \mathbf{\Omega}_\mathrm{s},\tag{28}
$$

with \mathbf{D}_0 the prescribed value of **D** at the point X_0 and Ω_s the following matricant

$$
\Omega_s = 1 + \int_0^s \mathbf{P}(\tau) d\tau + \int_0^s \left[\int_0^{\tau} \mathbf{P}(\tau_1) d\tau_1 \right] \mathbf{P}(\tau) d\tau + \dots, \tag{29}
$$

where 1 is the identity tensor. Since the right stretch tensor following from the polar decomposition theorem applied to D can be calculated from the strain tensor $C¹$, only three components ofthe rotation tensor should be prescribed at this point. Due to the integrability conditions (22) the solution **D** does not depend upon the choice of the curve $c(s)$. Therefore, if the body is simply connected, the solution for **D** presented by eqns (28) and (29) is unique up to a rigid body rotation.

Having determined **D**, we can easily get the deformation gradient F by multiplying (7) with D

$$
\mathbf{F} = \mathbf{D}\mathbf{H}.\tag{30}
$$

Assuming that **H**, $C¹$ and $T¹$ satisfy the compatibility condition (19), we multiply eqn (30) with the tangent vector $\dot{\mathbf{X}}$ of the curve $c(s)$ connecting two arbitrary points to get

$$
\frac{\mathrm{d}}{\mathrm{d}s}\mathbf{x} = \mathbf{D} \mathbf{H} \dot{\mathbf{X}}.\tag{31}
$$

Equation (32) yields the following solution

$$
\mathbf{x}(s) = \mathbf{x}_0 + \int_0^s \mathbf{D} \mathbf{H} \dot{\mathbf{X}} \, \mathrm{d}s. \tag{32}
$$

It is easy to check that, if the tensor field D is determined uniquely up to a rigid-body rotation, then x is determined by eqn (32) uniquely up to the rigid-body motion (with the same rotation tensor) for simply connected bodies.

4. PRINCIPLE OF VIRTUAL WORK

The formulation of the virtual work principle in the theory of oriented media depends essentially on the choice of the principal unknown functions. In the most natural setting we regard x and D as such unknown quantities subject to variation. We define the local virtual work in the following way

$$
\delta \mathscr{W}_1 = \int_{\mathscr{U}} (Ph, Grad\delta x > + Jl, \delta D > + Pl, Grad\delta D >) dv,
$$
 (33)

where $\langle \ldots \rangle$ denotes the pairing between dual tensors. We call P^h , J^I and P^l stresses, director stresses and microstresses, respectively. We postulate now the principle of virtual work in the form

$$
\delta \mathscr{W}_1 = \int_{\mathscr{U}} (\mathbf{B}^h \cdot \delta \mathbf{x} + \langle \mathbf{B}^l, \delta \mathbf{D} \rangle) dv + \int_{\partial \mathscr{U}} (\langle \mathbf{P}^h_{\nu}, \delta \mathbf{x} \rangle + \langle \mathbf{P}^l_{\nu}, \delta \mathbf{D} \rangle) da \tag{34}
$$

for arbitrary sub-bodies \mathcal{U} , with \mathbf{B}^h and \mathbf{B}^l the body macro- and microforce, and \mathbf{P}_v^h and \mathbf{P}_{u}^{\perp} the macro- and microtraction specified on the boundary $\partial \mathcal{U}$, respectively. Standard procedure leads to the following equations [cf. Capriz (1989)]

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$$
DivPh + Bh = 0,
$$
 (35)

$$
\mathbf{Div}\mathbf{P}^{\mathbf{I}} - \mathbf{J}^{\mathbf{I}} + \mathbf{B}^{\mathbf{I}} = 0,
$$
\n(36)

and boundary conditions

$$
\mathbf{P}^{\mathrm{h}}\mathbf{N}=\mathbf{P}_{\mathrm{v}}^{\mathrm{h}},\tag{37}
$$

$$
\mathbf{P}^{\mathrm{I}}\mathbf{N} = \mathbf{P}^{\mathrm{I}}_{\nu},\tag{38}
$$

Consider now the special case, when a function $W_1(\mathbf{F}, \mathbf{D}, \text{GradD})$ exists such that

$$
\delta \mathscr{W}_1 = \delta \int_{\alpha} W_1(\mathbf{F}, \mathbf{D}, \text{GradD}) \, \mathrm{d}v. \tag{39}
$$

The oriented media of the type (39) are called hyperelastic and the function $W_1(F, D, GradD)$ is called free energy density. In this case P^h , P^h and J^h are given by

$$
\mathbf{P}^{\mathrm{h}} = \frac{\partial W_1}{\partial \mathbf{F}} \bigg|_{\mathbf{D}, \text{GradD}}, \tag{40}
$$

$$
\mathbf{J}^1 = \frac{\partial W_1}{\partial \mathbf{D}}\bigg|_{\mathbf{F}, \text{GradD}},\tag{41}
$$

$$
\mathbf{P}^{\prime} = \frac{\partial W_1}{\partial \text{GradD}}\bigg|_{\mathbf{F}, \mathbf{D}},\tag{42}
$$

and the mechanical response is completely governed by this free energy density.

5. FRAME INDIFFERENCE

Let us consider the special case of hyperelastic oriented media, whose mechanical response is governed by the function $W_1(\mathbf{F}, \mathbf{D}, \mathbf{GradD})$. The stress state arising within bodies is produced as a result of strains leading to the energy stored. Therefore, if we superpose a rigid-body motion onto the actual motion of the body we must also expect $W_1(\mathbf{F}, \mathbf{D}, \mathbf{GradD})$ to remain unchanged. Such a scalar function is called frame indifferent.

Consider two motions ϕ (**X**, *t*), **D**(**X**, *t*) and ϕ ^{*}(**X**, *t*), **D**^{*}(**X**, *t*) of an oriented body. These motions are regarded as differing from one another by a rigid-body motion, if at any instant they are related by

$$
\boldsymbol{\phi}^*(\mathbf{X},t) = \mathbf{c}(t) + \mathbf{Q}(t)[\boldsymbol{\phi}(\mathbf{X},t) - \mathbf{x}_0],
$$
\n(43)

$$
\mathbf{D}^*(\mathbf{X},t) = \mathbf{Q}(t)\mathbf{D}(\mathbf{X},t),\tag{44}
$$

where $c(t)$ is a time-dependent point, $Q(t)$ is a time-dependent orthogonal tensor and x_0 is a fixed point. The precise meaning of eqn (44) is that if the rigid-body motion eqn (43) is applied to the underlying body, its directors in all points will rotate with *the same* Q.

When the rigid-body motion (43), eqn (44) is superposed, we have

$$
\mathbf{F}^* = \mathbf{Q}\mathbf{F},\tag{45}
$$

$$
GradD^* = QGradD.
$$
 (46)

A scalar function is said to be frame indifferent if it does not change its value when D, **F,** GradD are changed according to eqns (44)-(46). Now we want to show that if the free energy density is frame indifferent, it can depend only on H , $C¹$ and Γ .

Using the definitions $(7)-(11)$ one can see that

$$
H^* = D^{*-1}F^* = D^{-1}Q^{-1}QF = D^{-1}F = H,
$$
\n(47)

$$
\mathbf{C}^{1*} = \mathbf{D}^{*T} \mathbf{g} \mathbf{D}^{*} = \mathbf{D}^{T} \mathbf{Q}^{T} \mathbf{g} \mathbf{Q} \mathbf{D} = \mathbf{C}^{t},
$$
\n(48)

and

$$
\Gamma^* = \mathbf{D}^{*-1} \text{Grad} \mathbf{D}^*
$$

=
$$
\mathbf{D}^{-1} \mathbf{Q}^{-1} \mathbf{Q} \text{Grad} \mathbf{D} = \Gamma
$$
 (49)

hold. Hence, any scalar function depending on X , **H**, C^1 and Γ is frame indifferent.

Now let us consider two motions ϕ (**X**, *t*), **D**(**X**, *t*) and ϕ ^{*}(**X**, *t*), **D^{*}(X**, *t*) with the same strain measures $H = H^*$, $C^* = C^{\dagger}$ and $\Gamma = \Gamma^*$. We assume the following *local* relation between D and D* at the point X

$$
\mathbf{D}^* = \mathbf{Q}\mathbf{D},\tag{50}
$$

where Q is an arbitrary second rank tensor. From the condition $C^1 = C^{1*}$ it is easy to show that Q must be orthogonal. From the other two conditions, $H = H^*$ and $\Gamma = \Gamma^*$, one can show that the relations (45) and (46) are fulfilled. Thus, according to the principle of frame indifference the energy of these two motions should be the same so that we can write

$$
W = \hat{W}_1(\mathbf{H}, \mathbf{C}^1, \Gamma). \tag{51}
$$

We shall assume that the oriented material is homogeneous so that no explicit dependency of Won *X* is present.

Due to eqn (51) the constitutive eqns (40) and (41) become more specific. Let us find them out. Applying the rule of differentiation one gets easily

$$
(\mathbf{P}^{\mathrm{h}})_{\mathrm{a}}^{\mathrm{A}} = \frac{\partial \hat{W}_1}{\partial H_{\mathrm{A}}^{\mathrm{B}}} (\mathbf{D}^{-1})_{\mathrm{a}}^{\mathrm{B}}.
$$
 (52)

In order to calculate J^1 we use the following formulae

$$
\frac{\partial (\mathbf{D}^{-1})_b^{\mathbf{B}}}{\partial D_A^{\mathbf{A}}} = -(\mathbf{D}^{-1})_a^{\mathbf{B}} (\mathbf{D}^{-1})_b^{\mathbf{A}}
$$
(53)

$$
\frac{\partial \Gamma_{\text{CD}}^{\text{B}}}{\partial D_{\text{A}}^{\text{A}}} = -(\mathbf{D}^{-1})_{\text{a}}^{\text{B}} \Gamma_{\text{CD}}^{\text{A}}.
$$
\n(54)

Making use of the rule of differentiation one gets again

$$
(\mathbf{J}^{\mathsf{I}})^{\mathsf{A}}_{\mathsf{a}} = (\mathbf{D}^{-1})^{\mathsf{B}}_{\mathsf{a}} \Bigg[-\frac{\partial \hat{W}_{\mathsf{I}}}{\partial H^{\mathsf{B}}_{\mathsf{D}}} H^{\mathsf{A}}_{\mathsf{D}} + 2C^{\mathsf{I}}_{\mathsf{B}\mathsf{D}} \frac{\partial \hat{W}_{\mathsf{I}}}{\partial C^{\mathsf{I}}_{\mathsf{A}\mathsf{D}}} - \frac{\partial \hat{W}_{\mathsf{I}}}{\partial \Gamma^{\mathsf{B}}_{\mathsf{D}\mathsf{E}}} \Gamma^{\mathsf{A}}_{\mathsf{D}\mathsf{E}} \Bigg]. \tag{55}
$$

Similarly

Fig. 3. Multiplicative decomposition: (a) initial state; (b) deformed state; and (c) relaxed state (reference crystal).

$$
(\mathbf{P}^{\mathsf{I}})_{\mathsf{a}}^{\mathsf{A}\mathsf{B}} = (\mathbf{D}^{-1})_{\mathsf{a}}^{\mathsf{C}} \frac{\partial \tilde{W}_1}{\partial \Gamma_{\mathsf{B}\mathsf{A}}^{\mathsf{C}}}.
$$
 (56)

The fonnulae (52), (55) and (56) play the role of the constitutive equations in the theory of hyperelastic oriented continua.

6. APPLICATION TO CRYSTALS

It is well-known that dislocations, as bearers of the crystal defects, are responsible for the slip and the plastic defonnation of crystals and polycrystals. A continuum model of crystals (or polycrystals) [Bilby *et al.* (1955); Bilby *et al.* (1957); Kroner (1958,1960)] can be developed by identifying the triad of directors d_a with that of *lattice vectors* [cf. Naghdi and Srinivasa (1993, 1994)]. The deformation tensor D corresponds then to the lattice (elastic) deformation, which, in trend of the modern literature on finite elastoplasticity [see Le and Stumpf (1993, 1994) and the papers quoted therein], is frequently denoted by *Fe* as well[†]. Now let us consider a crystal undergoing nonhomogeneous plastic deformation and let us imaging the following thought experiment (Gedankenexperiment) : cut the defonned body into infinitesimal elements and reduce the stresses to zero. The stress-free elements will be called reference crystals. The fundamental assumption made by Bilby *et al. (1955,* 1957) and Kroner (1958, 1960) says that the elements are relaxed from the current state to this stress free state by the inverse lattice deformation D^{-1} . In its terms, the residual distortion tensor (7)

$$
\mathbf{H} = \mathbf{D}^{-1}\mathbf{F} = \mathbf{F}^{\mathbf{p}},\tag{57}
$$

will be called plastic deformation and denoted also by F^p . It is clear that H is a macroscopic quantity and has nothing to do with the lattice vectors. Figure 3 shows the local relations between different elements with their lattice vectors in the two-dimensional case.

Formula (57) corresponds to the multiplicative resolution of the total deformation. This resolution was first introduced by Bilby *et al.* (1957) as a basic assumption to derive the kinematics of crystals and polycrystals containing continuously distributed dislocations. In Bilby *et al.* (1957) F, D, H are called the shape, lattice and dislocation deformation, respectively. We adopt here the terminology used by Kröner (1958, 1960) and Lee (1969). The tensor \mathbf{C}^1 from eqn (9) (denoted also by $\mathbf{\bar{c}}^e$)

tIn Le and Stumpf (1994) the following component representation of the lattice deformation was used: $\mathbf{F}^e = (\mathbf{F}^e)^a_{\alpha} \mathbf{g}_a \otimes \mathscr{D}^a.$

Fig. 4. Definition of Burgers vector: (a) current configuration; (b) reference crystal.

$$
\mathbf{C}^1 = \mathbf{D}^T \mathbf{g} \mathbf{D} = \mathbf{\bar{c}}^c,\tag{58}
$$

will be called the elastic strain tensor.

It is clear that from $C¹$ alone one cannot determine **D** uniquely due to its incompatibility. Let us take now an arbitrary surface A bounded by a contour c in the current configuration and consider the integral

$$
\mathbf{b} = -\oint_{c} \mathbf{D}^{-1} \, \mathrm{d}\mathbf{x},\tag{59}
$$

which measures the incompatibility of the elastic deformation. If eqn (59) would vanish for all closed contours, then the director deformation could be presented as the gradient of a vector field. One can show that, in the limiting case of a continuum model (if we let the lattice constant approach zero), eqn (59) coincides with the resultant Burgers vector of all dislocations, whose dislocation lines intersect the surface *A.* The microscopic picture would look like Fig. 4.

Now let us apply Stokes' theorem to the contour integral (59)

$$
\mathbf{b} = -\int_{A} \mathbf{curl} \mathbf{D}^{-1} \mathbf{n} \, \mathrm{d}a,\tag{60}
$$

with **n** the normal vector to the surface A. For infinitesimal contours c we get from eqn (60)

$$
\mathbf{b} = \mathbf{x} \mathbf{n} \, \mathrm{d}a, \quad \mathbf{\alpha} = -\mathrm{curl} \mathbf{D}^{-1}.
$$
 (61)

The tensor α is called the dislocation density (see Fig. 5).

The dislocation density α and its associated tensor $(D^{-1})_{c,b}^A - (D^{-1})_{b,c}^A$ (which is skewsymmetric with respect to the covariant indices) are two-point tensors. Pulling back two leg of the latter with the help of D^{-1} gives

Fig. 5. Dislocation density tensor *ex.*

$$
(\mathbf{\bar{t}})_{\mathrm{BC}}^{\mathrm{A}} = D_{\mathrm{B}}^{\mathrm{b}} [(\mathbf{D}^{-1})_{\mathrm{c},\mathrm{b}}^{\mathrm{A}} - (\mathbf{D}^{-1})_{\mathrm{b},\mathrm{c}}^{\mathrm{A}}] D_{\mathrm{C}}^{\mathrm{c}}.
$$
\n(62)

This tensor can be interpreted as the torsion of the so-called crystal connection [see the geometric interpretation of this tensor in terms of the crystal connection in Le and Stumpf (1994)], One can also prove the following relation

$$
\left(\mathbf{\bar{t}}\right)_{\mathrm{BC}}^{\mathrm{A}} = \Gamma_{\mathrm{DB}}^{\mathrm{A}} (\mathbf{H}^{-1})_{\mathrm{C}}^{\mathrm{D}} - \Gamma_{\mathrm{DC}}^{\mathrm{A}} (\mathbf{H}^{-1})_{\mathrm{B}}^{\mathrm{D}}.
$$
\n(63)

Le and Stumpf (1994, 1996b) showed that, if the free energy per unit volume of the perfect crystal satisfies the principles of frame indifference and initial scaling indifference, it can depend only on \bar{c}^e and \bar{t}

$$
\omega = \hat{\omega}(\mathbf{\tilde{c}}^{\mathbf{e}}, \mathbf{\tilde{t}}). \tag{64}
$$

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

The formula (64) leads to the following free energy per unit initial volume

$$
W = \hat{W}_1(\mathbf{H}, \mathbf{C}^1, \Gamma) = J^p \hat{\omega}(\mathbf{\bar{c}}^c, \mathbf{\bar{t}}), \tag{65}
$$

with $J^p = det\mathbf{H}$, $\mathbf{\bar{c}}^e$ defined by eqn (58) and $\mathbf{\bar{t}}$ by (63). Making use of the formulae (52), (55) and (56) one gets the stresses

$$
(\mathbf{P}^{\mathrm{h}})_{\mathrm{a}}^{\mathrm{A}} = (\mathbf{D}^{-1})_{\mathrm{a}}^{\mathrm{B}} [\hat{W}_1 (\mathbf{H}^{-1})_{\mathrm{B}}^{\mathrm{A}} + J^{\mathrm{p}} (\mathbf{\bar{s}}^{\mathrm{d}})_{\mathrm{C}}^{\mathrm{DE}} \Gamma_{\mathrm{FE}}^{\mathrm{C}} (\mathbf{H}^{-1})_{\mathrm{B}}^{\mathrm{F}} (\mathbf{H}^{-1})_{\mathrm{D}}^{\mathrm{A}}],\tag{66}
$$

the director stresses

$$
(\mathbf{J}^{\mathbf{l}})^{\mathbf{A}}_{\mathbf{a}} = (\mathbf{D}^{-1})^{\mathbf{B}}_{\mathbf{a}} \left[-\hat{W}_{1} \delta^{\mathbf{A}}_{\mathbf{B}} - J^{p} (\mathbf{\bar{s}}^{\mathbf{d}})^{\mathbf{A}}_{\mathbf{C}} \Gamma^{C}_{\mathbf{D}E} (\mathbf{H}^{-1})^{\mathbf{D}}_{\mathbf{B}} + J^{p} (\mathbf{\bar{c}}^{\mathbf{e}})_{\mathbf{B}C} (\mathbf{\bar{s}})^{\mathbf{A}C} - J^{p} (\mathbf{\bar{s}}^{\mathbf{d}})^{\mathbf{E}F}_{\mathbf{D}E} \Gamma^{A}_{\mathbf{D}E} (\mathbf{H}^{-1})^{\mathbf{D}}_{\mathbf{F}} \right], \quad (67)
$$

and the microstresses

$$
(\mathbf{P}^I)^{AB}_{a} = J^p (\mathbf{D}^{-1})^C_a (\mathbf{\bar{s}}^d)^{AD}_{C} (\mathbf{H}^{-1})^B_D. \tag{68}
$$

The stresses \bar{s} and couple-stresses \bar{s}^d are given by

$$
(\mathbf{\bar{s}})^{\mathbf{AB}} = 2 \frac{\partial \hat{\omega}}{(\mathbf{\bar{c}}^{\mathbf{e}})_{\mathbf{AB}}},\tag{69}
$$

$$
(\bar{\mathbf{s}}^{\mathbf{d}})_{\mathbf{C}}^{\mathbf{A}\mathbf{B}} = 2 \frac{\partial \varphi}{(\bar{\mathbf{t}})_{\mathbf{A}\mathbf{B}}^{\mathbf{C}}}.
$$
 (70)

7. COMPARISON WITH FINITE ELASTOPLASTICITY WITH MICROSTRUCTURE

In the finite elastoplasticity with microstructure we regard x and H as the principal unknown functions subject to variation. The local virtual work is defined as follows

$$
\delta \mathscr{W}_2 = \int_{\mathscr{U}} (P, D\delta \mathbf{x}> + J, \delta \mathbf{H}> + Pd, Grad \delta \mathbf{H} >) dv.
$$
 (71)

Fig. 6. Physical meaning of the couple stresses.

The stress measures **P,** J and *pd* introduced here will be called the (first Piola-Kirchhoff) macrostress tensor, the configurational stress tensor and the couple stress tensor, respectively. Based on this form of the local virtual work Le and Stumpf (1994) postulated the following principle of virtual work

$$
\delta \mathscr{W}_2 = \int_{\mathscr{U}} (\mathbf{B} \cdot \delta \mathbf{x} + \langle \mathbf{B}^d, \delta \mathbf{H} \rangle) dv + \int_{\partial \mathscr{U}} (\langle \mathbf{P}_v, \delta \mathbf{x} \rangle + \langle \mathbf{P}_v^d, \delta \mathbf{H} \rangle) da, \tag{72}
$$

using x and H as independent unknown fields [see also Naghdi and Srinivasa (1994)]. From the variational principle (72) the following equilibrium equations and boundary conditions have been derived

$$
\text{Div}\mathbf{P} + \mathbf{B} = 0,\tag{73}
$$

$$
DivPd - J + Bd = 0,
$$
\n(74)

$$
PN = P_v, \t\t(75)
$$

$$
\mathbf{P}^{\mathrm{d}}\mathbf{N} = \mathbf{P}_{\mathrm{v}}^{\mathrm{d}}.\tag{76}
$$

The necessity of taking the couple stress into account can be clarified by the following example [Kröner (1960)]. Let us cut an element of a deformed beam. It may happen that dislocations, represented by the symbol \perp , are found near the boundary of this element (see Fig. 6). One can show then that a distribution of tractions is needed to keep all dislocations in equilibrium. From the microscopical point of view, these tractions are stresses, but from the macroscopical point of view, these are couple stresses.

The motion of dislocations is accompanied by the change of the configuration. This change is due to so-called configurational forces and configurational stresses J, respectively. **In** Fig. 7, four special cases of the configurational cases are indicated, where the case (d)

corresponds to the plastic deformation as a result of the motion of continuously distributed dislocations.

In the special case, when

$$
\delta \mathscr{W}_2 = \delta \int_{\mathscr{U}} W_2(\mathbf{F}, \mathbf{H}, \text{GradH}) \, \mathrm{d}v,\tag{77}
$$

the stress measures in eqns (73) and (74) are given by

$$
\mathbf{P} = \frac{\partial W_2}{\partial \mathbf{F}} \bigg|_{\mathbf{H}, \text{GradH}},
$$
\n(78)

$$
\mathbf{J} = \frac{\partial W_2}{\partial \mathbf{H}} \bigg|_{\mathbf{F}, \text{GradH}},
$$
\n(79)

$$
\mathbf{P}^{\mathbf{d}} = \frac{\partial W_2}{\partial \mathbf{GradH}_{\mathbf{F}, \mathbf{H}}}.
$$
 (80)

It can easily be shown that from (64) another equivalent form of the free energy per unit initial volume follows

$$
W = W_2(\mathbf{F}, \mathbf{H}, \text{GradH}), \tag{81}
$$

where

$$
W_2 = J^{\mathbf{p}} \hat{\boldsymbol{\omega}}(\mathbf{\bar{c}}^{\mathbf{e}}(\mathbf{F}, \mathbf{H}), \mathbf{\bar{t}}(\mathbf{H}, \mathbf{GradH})). \tag{82}
$$

Assuming that eqn (77) holds, one can derive the following constitutive equations in terms of W_2

$$
P_{\rm a}^{\rm A} = g_{\rm ab} F_{\rm B}^{\rm b} S^{\rm AB},\tag{83}
$$

$$
S^{AB} = Jp(\bar{\mathbf{s}})^{CD}(\mathbf{H}^{-1})^{\mathbf{A}}_{\mathbf{C}}(\mathbf{H}^{-1})^{\mathbf{B}}_{\mathbf{D}},
$$
(84)

$$
J_{\rm B}^{\rm A} = (H^{-1})_{\rm B}^{\rm C}[-C_{\rm CD}S^{\rm DA} + W_2\delta_{\rm C}^{\rm A} + T_{\rm CD}^{\rm E}(S^{\rm d})_{\rm E}^{\rm DA}]
$$
(85)

$$
(\mathbf{P}^d)_C^{AB} = -(\mathbf{H}^{-1})_C^D (\mathbf{S}^d)_D^{AB}
$$
 (86)

$$
(\mathbf{S}^{\mathbf{d}})_{\mathbf{C}}^{\mathbf{AB}} = J^{\mathbf{p}}(\mathbf{\bar{s}}^{\mathbf{d}})_{\mathbf{F}}^{\mathbf{DE}} H_{\mathbf{C}}^{\mathbf{F}}(\mathbf{H}^{-1})_{\mathbf{D}}^{\mathbf{A}}(\mathbf{H}^{-1})_{\mathbf{E}}^{\mathbf{B}},\tag{87}
$$

where

$$
T_{BC}^A = (H^{-1})^A_D (H_{CB}^D - H_{BC}^D).
$$

Let us establish now the relationship between the stress measures P , J, P^d , given here with the stress measures P^h , J^l , P^l of Section 5 in the special case of hyperelastic oriented media with the free energy density (64). We substitute $\mathbf{D} = \mathbf{F} \mathbf{H}^{-1}$ (from eqn (57)) into the local virtual work (33). After summing up terms with the same variations δx , δH and $D\delta H$ and comparing with the local virtual work (71) we get

$$
P_{a}^{A} = (P^{h})_{a}^{A} + (J^{l})_{a}^{B}(H^{-1})_{B}^{A} - (P^{l})_{a}^{EB}H_{D,B}^{C}(H^{-1})_{C}^{A}(H^{-1})_{E}^{D},
$$
\n(88)

$$
J_{\rm B}^{\rm A} = -({\bf J}^{\rm I})_{\rm a}^{\rm C} D_{\rm B}^{\rm a}({\bf H}^{-1})_{\rm C}^{\rm A} - ({\bf P}^{\rm I})_{\rm a}^{\rm CD} D_{\rm B,D}^{\rm a}({\bf H}^{-1})_{\rm C}^{\rm A} + ({\bf P}^{\rm I})_{\rm a}^{\rm C} D_{\rm B}^{\rm a} H_{\rm D,E}^{\rm F}({\bf H}^{-1})_{\rm C}^{\rm D}({\bf H}^{-1})_{\rm F}^{\rm A}.
$$
 (89)

and

$$
(\mathbf{P}^d)_C^{AB} = -(\mathbf{P}^l)_a^{DB} F_E^a (\mathbf{H}^{-1})_C^E (\mathbf{H}^{-1})_D^A.
$$
 (90)

It can be proved, by direct calculation, that eqns (35) – (38) and (73) – (76) are equivalent. provided the microtraction on the boundary is zero and the body forces, body microforces and boundary tractions in eqns (34) and (72), respectively, are interrelated by

 $\bar{\mathcal{A}}$

$$
B_{a} = (B^{h})_{a} - ((B^{l})_{a}^{A}(H^{-1})_{A}^{B})_{B}, \qquad (91)
$$

$$
(\mathbf{B}^d)_\mathbf{B}^\mathbf{A} = -((\mathbf{B}^l)_a^C D_\mathbf{B}^\mathbf{a} (\mathbf{H}^{-1})_C^\mathbf{A},\tag{92}
$$

$$
(\mathbf{P}_{\nu})_a = (\mathbf{P}_{\nu}^{\mathrm{h}})_a + ((\mathbf{B}^{\mathrm{l}})_a^{\mathrm{A}} (\mathbf{H}^{-1})_A^{\mathrm{B}} N_{\mathrm{B}}.\tag{93}
$$

Note that this equivalence is no longer valid, if the microtraction P_t on the boundary does not vanish. In that case the boundary condition cannot be reduced to that of eqn (76).

8. CONCLUSIONS

There are two different approaches to the model of oriented continua. Toupin (1964), Capriz and Podio-Guidugli (1976) and Capriz (1989) consider the displacement and the director deformation fields as the primary unknown functions, which should be subject to variation in the principle of virtual work. Alternatively, Le and Stumpf (1994, 1996a,b,c) and Naghdi and Srinivasa (1993, 1994) take the displacement and the microdeformation (plastic deformation) fields as the primary unknown functions subject to variation. We have shown that if the microtraction on the boundary is zero, these two theories are equivalent within the elastic range given by eqn (64). Despite this fact, the latter approach leads to the clear and physically tractable stress measures eqns (83)–(87) so that it is more convenient to use them instead of those defined in eqns (66) – (68) .

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