Extending Teodosiu's models within the finite elasto-plasticity constitutive framework

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Abstract :

The paper is devoted to elasto-plastic models for crystalline materials within the constitutive framework of non-local crystalline plasticity and crystalline elasto-plastic materials with microstructural defects, respectively. A non-local crystal plasticity model based on a multi-slip flow rule, coupled with diffusion like evolution equations for scalar dislocation densities, with hardening influenced by dislocations and the back stress involved in the activation condition is presented. The geometrical non-Riemannian structure of the material space which is associated with an elasto-plastic crystalline material with defects at the lattice level, is characterized and discussed in terms of connections with non-zero torsion and non-zero curvature.

Mots clefs : multiplicative decomposition, elasto-plastic, crystalline materials, flow rule, defects, connection and torsion, evolution equations.

1 Introduction

We propose and analyze elasto-plastic models for crystalline materials as extension of Teodosiu's models in two directions : non-local crystal plasticity and crystalline elasto-plastic materials with microstructural defects. Kröner and Teodosiu [1] argue that plasticity and viscoplasticity are typical properties of crystalline materials, which are generated by existing inside defects. Lattice continuous defects have been defined using the differential geometry approaches by de Wit [2] (in a linear approximation), Kondo and Yuki [3], Kröner [4]. Following Kröner [5], the geometrical non-Riemannian structure of the material space, associated with an elasto-plastic crystalline material with defects at the lattice level, is characterized by a connection with non-zero torsion and non-zero curvature.

Teodosiu [6] introduced the concept of local, relaxed (stress free), isoclinic configurations in order to define correctly the elastic and plastic parts of the deformation gradient, called *elastic and plastic distortions*. The elastic distortion is a measure of deformation of crystalline lattice, while the plastic is associated with an unsltressed state. Thus the (anholonomic) deformation gradient is multiplicatively decomposed into elastic and plastic components. Material response is elastic with respect to the isoclinic configurations, while the plastic distortion and internal variables are defined by the appropriate

evolution equations, see also Teodosiu and Sidoroff [7], as well as Cleja-Ţigoiu and Soós [8] for the material symmetry concept. In section 2.1, as a natural generalization of the models developed by Teodosiu et al. [9], Cleja-Ţigoiu and Paşcan [10] proposed a crystal plasticity model based on a multi-slip flow rule, coupled with diffusion like evolution equations for scalar dislocation densities, with hardening influenced by dislocations and the back stress involved in the activation condition dependent on the gradients of dislocation densities. The variational formulation of the boundary value problem is provided in section 2.2.

In section 3 we introduce two types of models for crystalline elasto-plastic materials with microstructural defects. We shortly present here certain fundamental results that will be useful in describing the behaviour of elasto-plastic materials with structural defects in section 3.1. For mathematical concepts about affine connections on manifolds and geometry of Riemann-Cartan manifolds see Schouten [11], Clayton [12], Yavari [13]. We follow the presentation from Cleja-Ţigoiu and Ţigoiu [14].

Teodosiu [15] -[17] developed an elastic type theory of materials with initial stresses and hyperstresses induced by dislocations, see section 3.2. In section 3.3 we discuss certain aspects related to the elastoplastic models proposed by Cleja-Ţigoiu [18], Cleja-Ţigoiu et al. [19] and [20]. These papers aim : to describe the behaviour of crystalline materials containing defects by non-local fields that are smooth over an interatomic length scale and at the time of micro-seconds ; to elaborate a strategy to solve the initial boundary value problems for elasto-plastic materials with defects, such as dislocations, disclinations and grain boundaries ; to propose the algorithms to simultaneously solve the incremental equilibrium equation, coupled with partial differential equations which describe the defects evolution.

2   Non-local crystal plasticity

Teodosiu [6] assumes that, at least in principle, for any material point X a neighborhood $\mathcal{N}_X$ can be cut out from the body and relax it (which means that the macroscopic stress is vanishing) maintaining the position and values of dislocations within $\mathcal{N}_X$. The local relaxed configurations are defined to within a rigid rotation. Since the elastic reversible deformation represents the deformation of the crystalline lattice the indetermination in choosing the relaxed configuration has to be eliminated. By assuming that in all local relaxed configurations of $\mathcal{N}_X$ the crystalline directions are parallel to each other these configurations, called *isoclinic*, are uniquely defined relatively a fixed reference configuration, apart from the orthogonal maps, which are elements of the material symmetry group.

2.1   Slip systems and dislocations

We shortly present the crystal plasticity model proposed by Cleja-Ţigoiu and Paşcan [10]. The model generalizes the model developed by Teodosiu et al. [9], it is based on the multiplicative decomposition and on multi-slip flow rule.

Axiom The deformation gradient $\mathbf{F} = \nabla\chi(\cdot, t)$, associated with the motion, χ, of the body $\mathcal{B}$, is multiplicatively decomposed into elastic and plastic components, $\mathbf{F}^e$ and $\mathbf{F}^p$, given by

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p, \tag{1}$$

As a direct consequence of the multiplicative decomposition of the deformation gradient the velocity gradient, $\mathbf{L} = \dot{\mathbf{F}}\,\mathbf{F}^{-1}$ relates to the rate of plastic distortion, $\mathbf{L}^p$, and the rate of elastic distortion, $\mathbf{L}^e$,

through

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e \, \mathbf{L}^p \, (\mathbf{F}^e)^{-1}, \quad \mathbf{L}^e = \dot{\mathbf{F}}^e \, (\mathbf{F}^e)^{-1}, \quad \mathbf{L}^p = \dot{\mathbf{F}}^p \, (\mathbf{F}^p)^{-1}. \tag{2}$$

Axiom Material response is elastic with respect to the isoclinic configurations expressed either by

$$\frac{\boldsymbol{\Pi}}{\tilde{\rho}} = \mathcal{C}[\frac{1}{2} \, (\mathbf{C}^e - \mathbf{I})], \quad \text{where} \quad \mathbf{C}^e = (\mathbf{F}^e)^T \mathbf{F}^e \tag{3}$$

in terms of Piola-Kirchhoff stress tensor $\boldsymbol{\Pi}$, or in the actual configuration expressed in terms of Cauchy stress, $\mathbf{T}$, through

$$\frac{\mathbf{T}}{\hat{\rho}} = \mathbf{F}^e \mathcal{C}[\frac{1}{2} \, (\mathbf{C}^e - \mathbf{I})](\mathbf{F}^e)^T. \tag{4}$$

The elastic compliance matrix in the actual configuration, $\mathcal{E}$, is derived from the matrix of the elastic material, $\mathcal{C}$, with the constant coefficients given with respect to an isoclinic (i.e. lattice) configuration by the pushing away procedure, namely

$$\mathcal{E}[\mathbf{X}] = \mathbf{F}^e(\mathcal{C}\left[(\mathbf{F}^e)^T \mathbf{X} \mathbf{F}^e\right])(\mathbf{F}^e)^T, \quad \forall \, \mathbf{X} \text{ a symmetric tensor.} \tag{5}$$

In the paper $\tilde{\rho}$, $\hat{\rho}$ and $\hat{\rho}_0$ denote mass densities with respect to the lattice configuration, current and reference configurations, respectively.

Axiom The evolution in time of the plastic distortion is described by multi-slips in the appropriate crystallographic system (i.e. in the isoclinic configuration) as given by Kroöner and Teodosiu [1]

$$\dot{\mathbf{F}}^p \, (\mathbf{F}^p)^{-1} = \sum_{\alpha=1}^{N} \nu^\alpha (\bar{\mathbf{s}}^\alpha \otimes \bar{\mathbf{m}}^\alpha), \tag{6}$$

where ν^α are the plastic shear rates in the slip system α, $\bar{\mathbf{m}}^\alpha$ is the normal to the slip plane and $\bar{\mathbf{s}}^\alpha$ is the slip direction.

In the actual configuration the slip system, $(\mathbf{m}^\alpha, \mathbf{s}^\alpha)$, is defined by the formulae

$$\mathbf{s}^\alpha = \mathbf{F}^e \bar{\mathbf{s}}^\alpha, \quad \mathbf{m}^\alpha = (\mathbf{F}^e)^{-T} \, \bar{\mathbf{m}}^\alpha. \tag{7}$$

Theorem. *Rate form of the adopted constitutive framework by Cleja-Ţigoiu and Paşcan [10] : The differential system which defines the unknowns* $\mathbf{T}/\rho, \mathbf{F}^e, \gamma^\alpha, \mathbf{s}^\alpha, \mathbf{m}^\alpha, \zeta^\alpha \rho^\alpha$ *is given in the following form*

written below for a given history of the deformation gradient, $t \rightarrow \mathbf{F}(t), t \in [t_0, t^*)$:

$$\frac{d}{dt}\left(\frac{\mathbf{T}}{\hat{\rho}}\right) = \mathbf{L}\frac{\mathbf{T}}{\hat{\rho}} + \frac{\mathbf{T}}{\hat{\rho}}\mathbf{L}^T + \mathcal{E}\left[\mathbf{D}\right] - \sum_{\alpha=1}^{N}\nu^{\alpha}\mathcal{E}\left[\{\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}\}^{\mathsf{S}}\right] -$$

$$-\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}\right)\frac{\mathbf{T}}{\hat{\rho}} - \frac{\mathbf{T}}{\hat{\rho}}\sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}\right)^T$$

$$\dot{\mathbf{F}}^e\left(\mathbf{F}^e\right)^{-1} = \mathbf{L} - \sum_{\alpha=1}^{N}\nu^{\alpha}\left(\mathbf{s}^{\alpha} \otimes \mathbf{m}^{\alpha}\right)$$

$$\dot{\gamma}^{\alpha} = \frac{\hat{\rho}_0}{\hat{\rho}}\dot{\gamma}_0^{\alpha}\left|\frac{1}{\zeta^{\alpha}}(\mathbf{T}\mathbf{m}^{\alpha} \cdot \mathbf{s}^{\alpha} - \tau_b^{\alpha})\right|^n sign\left(\mathbf{T}\mathbf{m}^{\alpha} \cdot \mathbf{s}^{\alpha} - \tau_b^{\alpha}\right)\mathcal{H}\left(\mathcal{F}^{\alpha}\right) , \alpha = 1, \ldots, N$$

$$\tau_b^{\alpha} = \kappa_2(\bar{\mathbf{s}}^{\alpha} \cdot \nabla\rho^{\alpha})(\bar{\mathbf{m}}^{\alpha} \cdot \nabla\rho^{\alpha})$$

(8)

where $\nu^{\alpha} = \dot{\gamma}^{\alpha}$,

$$\dot{\mathbf{s}}^{\alpha} = \mathbf{L}\mathbf{s}^{\alpha} - \sum_{\beta=1}^{N}\nu^{\beta}\left(\mathbf{s}^{\beta} \otimes \mathbf{m}^{\beta}\right)\mathbf{m}^{\alpha}, \quad \alpha = 1, \ldots, N$$

$$\dot{\mathbf{m}}^{\alpha} = -\mathbf{L}^T\mathbf{m}^{\alpha} + \sum_{\beta=1}^{N}\nu^{\beta}\left(\mathbf{m}^{\beta} \otimes \mathbf{s}^{\beta}\right)\mathbf{m}^{\alpha}, \alpha = 1, \ldots, N$$

(9)

$$\dot{\zeta}^{\alpha} = \sum_{\beta=1}^{N}h^{\alpha\beta}\left|\dot{\gamma}^{\beta}\right|, \quad \alpha = 1, \ldots, N$$

There are considered either a local evolution equation for the dislocation density

$$\dot{\rho}^{\alpha} = \frac{1}{b}\left(\frac{1}{L^{\alpha}} - 2y_c\rho^{\alpha}\right)|\nu^{\alpha}|, \quad L^{\alpha} = K\left(\sum_{q \neq \alpha}\rho^q\right)^{-1/2}$$

(10)

or a non-local one

$$\dot{\rho}^{\alpha} = D|\nu^{\alpha}|\left(k\Delta\rho^{\alpha} - \frac{\partial\psi_T}{\partial\rho^{\alpha}}\right), \quad \alpha = 1, \ldots, N.$$

(11)

The yield function $\mathcal{F}^{\alpha}$, *which enters the activation condition* $\mathcal{F}^{\alpha} \geq 0$ *via the Heaviside function involved in the expression of the plastic shear rates is defined as*

$$\mathcal{F}^{\alpha}(\mathbf{T}, \mathbf{s}^{\alpha}, \mathbf{m}^{\alpha}, \zeta^{\alpha}, \rho^{\alpha}, \nabla\rho^{\alpha}) := |\frac{1}{\zeta^{\alpha}}(\tau^{\alpha} - \tau_b^{\alpha})| - \zeta^{\alpha},$$

(12)

were $\tau^{\alpha} = \mathbf{T}\mathbf{m}^{\alpha} \cdot \mathbf{s}^{\alpha}$ *is the effective reduced shear stress.*

The *initial conditions have to be attached to the differential system*, as well as as a *boundary value*

problem has to be defined in connection with the partial differential equation (10).

Boundary conditions : Solving the equilibrium problem for viscoplastic crystalline materials, containing dislocations, the macro boundary conditions which traditionally describe the traction and velocity have to be completed with micro boundary conditions in order to accurately describe the nature of the plastic deformation at micro-scale, from a physical point of view. From mathematical point of view the integration of the system of partial differential equations requires additional boundary conditions.

We remark that Teodosiu [6] mentioned that the shear rate is expressed by $\dot{\gamma}^\alpha = b^\alpha \; \alpha_M^\alpha \; v^\alpha$, which means that it depends on the magnitude of the Burgers vector, on the total length of mobile dislocation and the mean velocity of dislocation loop.

Comments of the model proposed by Cleja-Ţigoiu and Paşcan [10] :

- The evolution equation for ζ^α, i.e. the hardening law, is described in terms of the hardening matrix represented by Teodosiu et al. [9]

- The *viscoplastic flow* rule associated with the deformation process is given in the form similar to those introduced by Teodosiu and Sidoroff [7], but back stress not being included.

- The evolution equation (10) is given by Mecking and Kocks [22] and a diffusive evolution equation of the type (11) is considered by Bortoloni and Cermelli [23]. Herein an appropriate expression for the potential ψ_T is identified by considering the equality between the functions in the right hand side of equations (10) and (11) with $k = 0$.

- The expression of the back stress involved in the activation for $\alpha-$ slip system is proposed by Cleja-Ţigoiu and Paşcan [21] (within the constitutive framework developed by Cleja-Ţigoiu [24]) to be given by

$\tau_b^\alpha = \mathrm{div}(\kappa_3 \; \bar{\mathbf{m}}^\alpha \times (\boldsymbol{\alpha}_N)^T \; \bar{\mathbf{s}}^\alpha) + \kappa_2(\bar{\mathbf{s}}^\alpha \cdot \nabla\rho^\alpha)(\bar{\mathbf{m}}^\alpha \cdot \nabla\rho^\alpha)$. As a particular case, namely for $\kappa_3 = 0$, the expression of the back stress follows

$$\tau_b^\alpha = \kappa_2(\bar{\mathbf{s}}^\alpha \cdot \nabla\rho^\alpha)(\bar{\mathbf{m}}^\alpha \cdot \nabla\rho^\alpha). \tag{13}$$

2.2 Variational problem

The weak formulation associated with the balance equations at time t can be emphasized using an update Lagrangian formalism (see Cleja-Ţigoiu [25], or a principle of the virtual power, see Teodosiu et al. [9].

First we derive the rate quasistatic boundary value problem associated with a generic stage of the process, following Cleja-Ţigoiu and Matei [25]. We use the *relative description of the motion* χ, given by Truesdell and Noll [26].

The nominal stress (i.e. the first Piola-Kirchhoff stress tensor) with respect to the configuration at time t is given by

$$\mathbf{S}_t(\mathbf{x}, \tau) = (\mathrm{det}\mathbf{F}_t(\mathbf{x}, \tau))\, \mathbf{T}(\mathbf{y}, \tau)\, (\mathbf{F}_t(\mathbf{x}, \tau))^{-T}, \quad \mathrm{det}\mathbf{F}_t(\mathbf{x}, \tau) = \frac{\hat{\rho}(\mathbf{x}, t)}{\hat{\rho}(\mathbf{y}, \tau)}. \tag{14}$$

Proposition.*1. The nominal stress satisfies, at moment t, the following relations*

$$\mathbf{S}_t\left(\mathbf{x}, t\right) = \mathbf{T}\left(\mathbf{x}, t\right) \quad and$$

(15)

$$\dot{\mathbf{S}}_t\left(\mathbf{x}, t\right) = \hat{\rho}\left(\mathbf{x}, t\right) \frac{d}{dt}\left(\frac{\mathbf{T}\left(\mathbf{x}, t\right)}{\hat{\rho}\left(\mathbf{x}, t\right)}\right) - \mathbf{T}\left(\mathbf{x}, t\right) \mathbf{L}^T\left(\mathbf{x}, t\right).$$

2. The Piola - Kirchhoff (nominal stress) $\mathbf{S}_t$ satisfies the balance equation with respect to the configuration at time t taken as reference configuration

$$div_{\mathbf{x}}\mathbf{S}_t\left(\mathbf{x}, \tau\right) + \hat{\rho}\left(\mathbf{x}, \tau\right) \mathbf{b}_t\left(\mathbf{x}, \tau\right) = 0, \quad with \quad \mathbf{b}_t\left(\mathbf{x}, \tau\right) = \mathbf{b}\left(\chi_t\left(\mathbf{x}, \tau\right), \tau\right).$$

(16)

The body is identified with $\Omega \subset \mathbf{R}^3$ and the appropriate boundary conditions are associated on the boundary $\partial\Omega_t$ of the current domain $\Omega_t = \chi(\Omega, t)$.

Now we emphasize an explicit representation of the variational equation associated with the rate form of the equilibrium equation at a current moment of time, (16) together with (22) in terms of the velocity in the actual configuration.

Theorem. *If the activation condition is formulated, the rate type boundary value problem at time t leads to an appropriate variational equality to be satisfied by the velocity field, $\mathbf{v}$, when the current state of the body, namely the Cauchy stress, $\mathbf{T}$, the position of the slip systems, $(\mathbf{m}^\alpha, \mathbf{s}^\alpha)$, the dislocation densities, ρ^α, the mass density $\hat{\rho}$, and the hardening variables, ζ^α, are known. The variational equality is given by*

$$\int_{\Omega_t} (\nabla\mathbf{v})\mathbf{T} \cdot \nabla\mathbf{w} d\, V + \int_{\Omega_t} \hat{\rho}\mathcal{E}[\mathbf{D}] \cdot \nabla\mathbf{w} d\, V -$$

$$- \sum_{\alpha=1}^{N} \int_{\Omega_t} \nu^\alpha \{\hat{\rho}\mathcal{E}\left[\{\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha\}^{\mathsf{S}}\right] + (\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)\,\mathbf{T} + \mathbf{T}\,(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha)^T\} \cdot \nabla\mathbf{w} d\, V = \qquad (17)$$

$$= \int_{\Gamma_{1t}} \dot{\mathbf{s}}_t \cdot \mathbf{w} da + \int_{\Omega_t} \rho\dot{\mathbf{b}}_t \cdot \mathbf{w} d\, V, \quad \forall \mathbf{w} \in \mathcal{V}_{ad},$$

with

$$\nu^\alpha = J\,\nu_0^\alpha\left|\frac{1}{\zeta^\alpha}(\mathbf{T}\mathbf{m}^\alpha \cdot \mathbf{s}^\alpha - \tau_b^\alpha)\right|^n sign\left(\mathbf{T}\mathbf{m}^\alpha \cdot \mathbf{s}^\alpha - \tau_b^\alpha\right)\mathcal{H}\left(\mathcal{F}^\alpha\right), \quad \alpha = 1, \dots, N \qquad (18)$$

A novel algorithm to describe the behaviour of the elasto-plastic body, at a generic time t is proposed : We apply the variational equality (17), (18) together with the differential equations which allow us to update the state of the material, to the sheet in a plane stress state.

A finite element method (FEM) is applied for solving the variational problem (17) to define the velocity field in the actual configuration, $\mathbf{v}$;

If the velocity field is known the solution of the differential system (which defines the rate type of the constitutive equations) and of the non-local evolution equation for the dislocation density (if this is the case) are solved to update the current sktate. We use Euler method and also Crank-Nicolson's method for non-local evolution equation.

3 Crystalline elasto-plastic materials with microstructural defects

Three configurations are considered in the paper :

– k be a fixed reference configuration of the body $\mathcal{B}$, i.e. a diffeomorphism, $k(\mathcal{B}) \subset \mathcal{E}$, and $\mathcal{B}$ will be identified with $k(\mathcal{B})$;

– $\chi(\cdot, t)$ the deformed configuration at time t, for any motion of the body $\mathcal{B}$, $\chi : \mathcal{B} \times R \longrightarrow E$,

– there exists $\mathcal{K}$, a time dependent anholonomic configuration (so-called configuration with torsion), defined by the pair $(\mathbf{F}^p, \overset{(p)}{\boldsymbol{\Gamma}})$, $\mathbf{F}^p-$ plastic distortion and $\overset{(p)}{\boldsymbol{\Gamma}}$ − plastic connection.

The plastic distorsion, $\mathbf{F}^p$, is an invertible second order tensor field and the plastic connection with torsion, $\overset{(p)}{\boldsymbol{\Gamma}}_k$, is a (1,2) third order tensor field attached to the configuration κ. The reference configuration k has not been mentioned anymore.

3.1 Connection with torsion, contorsion

In this section we introduce the definition, properties and axioms, concerning the connection with metric property with respect to a given metric, which is characterized by a positive and symmetric tensorial field defined on the body $\mathcal{B}$, starting from the results previously mentioned.

Definition. The so-called *motion connection* $\boldsymbol{\Gamma}$ is a compatible connection attached to the tensorial field $\mathbf{F} = \nabla\chi$, i.e. deformation gradient, as

$$\boldsymbol{\Gamma} = \mathbf{F}^{-1}(\nabla\,\mathbf{F}). \tag{19}$$

Let $\boldsymbol{\Gamma}$ be a connection and $\mathbf{C}$ a metric tensor, i.e. a symmetric and positive definite second order tensor.

Definition. The connection $\boldsymbol{\Gamma}$ has the **metric property** relative to the metric tensor, $\mathbf{C}$, or it is $\mathbf{C}-$ metric, if the following equality holds

$$(\nabla\,\mathbf{C})\mathbf{u} = (\boldsymbol{\Gamma}\mathbf{u})^T\mathbf{C} + \mathbf{C}(\boldsymbol{\Gamma}\mathbf{u}), \tag{20}$$

for any constant vector $\mathbf{u}$.

Remark. The precise meaning of (20) is given by the statement : the covariant derivative of *the metric tensor* $\mathbf{C}$ relative to the affine connection $\boldsymbol{\Gamma}$ is vanishing. The notation will be $\nabla_{\boldsymbol{\Gamma}}\mathbf{C} = 0$.

Definition. The torsion $\mathbf{S}$ of the connection $\boldsymbol{\Gamma}$ is defined by

$$(\mathbf{S}\mathbf{u})\mathbf{v} = (\boldsymbol{\Gamma}\mathbf{u})\mathbf{v} - (\boldsymbol{\Gamma}\mathbf{v})\mathbf{u}, \tag{21}$$

written for $\mathbf{u}, \mathbf{v} \in \mathcal{V}$.

We recall here Schouten's result [11] :

Theorem. *The connection $\boldsymbol{\Gamma}$, which is compatible with the metric tensor $\mathbf{C}$, is expressed in terms of Levi-Civita connection and contorsion $\mathbf{W}$ under the form*

$$\boldsymbol{\Gamma} = \boldsymbol{\gamma} + \mathbf{W}, \tag{22}$$

where

1. $\boldsymbol{\gamma}$ is Levi-Civita connection corresponding to the metric tensor $\mathbf{C}$ and is defined by the formula

$$(\boldsymbol{\gamma}\mathbf{u})\mathbf{v} \cdot \mathbf{w} = \frac{1}{2}\mathbf{C}^{-1}\mathbf{w} \cdot [((\nabla \mathbf{C})\mathbf{v})\mathbf{u} + ((\nabla \mathbf{C})\mathbf{u})\mathbf{v}] - \frac{1}{2}\nabla \mathbf{C}((\mathbf{C}^{-1})\mathbf{w})\mathbf{u} \cdot \mathbf{v}, \tag{23}$$

2. The contortion $\mathbf{W}$ and the torsion $\mathbf{S}$, third order fields, determine each other by

$$(\mathbf{Wu})\mathbf{v} = \frac{1}{2}(\mathbf{Su})\mathbf{v} - \frac{1}{2}\mathbf{C}^{-1}[(\mathbf{C}(\mathbf{Sv}))^T\mathbf{u} + (\mathbf{C}(\mathbf{Su}))^T\mathbf{v}],$$
$$(\mathbf{Su})\mathbf{v} = (\mathbf{Wu})\mathbf{v} - (\mathbf{Wv})\mathbf{u}. \tag{24}$$

3. The following skew-symmetries hold

$$(\mathbf{Su})\mathbf{v} = -(\mathbf{Sv})\mathbf{u},$$

$$(\bar{\mathbf{W}}\mathbf{u})^T = -(\bar{\mathbf{W}}\mathbf{u}), \quad where \quad \bar{\mathbf{W}} = \mathbf{CW}, \tag{25}$$

$\forall\, \mathbf{u}, \mathbf{v} \in \mathcal{V}$, *as a consequence of the definition of the torsion $\mathbf{S}$, (21).*

Let us give the component representations of the tensorial fields defined above in $\{x^i\}_{\{i=1,2,3\}} -$ a curvilinear coordinate system.

The following tensorial representations in local basis $\{\mathbf{e}^p\}_{p=1,2,3}$, and in the reciprocal basis $\{\mathbf{e}^p\}^{p=1,2,3}$, respectively, follow

$$\boldsymbol{\gamma} \equiv \gamma^p_{km}\mathbf{e}_p \otimes \mathbf{e}^k \otimes \mathbf{e}^m, \quad \gamma^p_{km} = \frac{1}{2}C^{pl}\left(\frac{\partial C_{lm}}{\partial x^k} + \frac{\partial C_{kl}}{\partial x^m} - \frac{\partial C_{km}}{\partial x^l}\right),$$

$$\mathbf{C}^{-1} = C^{pl}\mathbf{e}_p \otimes \mathbf{e}_l, \quad \mathbf{C} = C_{pl}\mathbf{e}^p \otimes \mathbf{e}^l, \quad \text{and} \quad C^{pl}C_{lm} = \delta^p_m,$$

$$(\nabla\mathbf{C})\mathbf{v} = \frac{\partial C_{sk}}{\partial x^k}v^l\mathbf{e}^s \otimes \mathbf{e}^k, \quad \text{where} \quad \mathbf{e}^p \cdot \mathbf{e}_m = \delta^p_m, \tag{26}$$

$$\boldsymbol{\Gamma} = \Gamma^k_{ij}\mathbf{e}_k \otimes \mathbf{e}^i \otimes \mathbf{e}^j, \quad ((\boldsymbol{\Gamma}\mathbf{u})\mathbf{v})\mathbf{w} = \Gamma^k_{ij}w_k u^j v^i,$$

$$\Gamma^k_{\nu\mu} = \gamma^k_{\nu\mu} + W^k_{\nu\mu},$$

$$W^k_{lm} = \frac{1}{2}[S^k_{lm} - C^{ks}(C_{mn}S^n_{sl} + C_{ln}S^n_{sm}],$$

$\gamma^p_{km} -$ second order Christoffel- Riemann symbols, $W^k_{\nu\mu} -$ contorsion components.

3.2 Teodosiu's elastic type models with dislocations

Elastic boundary value problems for defective bodies have several formulations, motivated by the adopted definitions for defects. The historical references to the elastic mathematical theory of dislocations and disclinations can be found for instance in Teodosiu [27]. Teodosiu formulated and solved boundary value problems for "Elastic models of crystalline defects" within small strain linear elasticity. **Elastic problems for defects characterized by Volterra process** have been solved by Teodosiu [27], as for instance the elastic model of the edge and screw dislocations in a hollow cylinder. In these problems the *given discontinuity* of the displacement field along the cut surface $\mathcal{S}$ characterizes the Burgers vector.

Teodosiu published "Contributions to continuum theory of dislocations and initial stresses, I-III," (1967),

Rev. Roum. Sci. Tech. [15], [16] and [17]. Herein a theory of materials with initial stresses and hyper-stresses induced by dislocations is developed. The considered second grade hyperelastic materials with strain energy dependent on the non-compatible elastic distortion and its covariant derivative generalizes the theory developed by Toupin [28]. The quasi-dislocations (described by the torsion tensor associated with a metric connection) are the only sources of the initial stresses and hyperstresses.

We refer now to Teodosiu's concepts, which deals with *natural state geometry*. The vanishing initial stresses is assumed to be performed by "tearing of the continuum body" into small elements and by "re-laxing them individually." Here a primary concept which further leads to isoclinic relaxed configuration seems to appear. These torn relaxed elements are considered as *imbedded in a metric space with linear connection*. Teodosiu points out that the natural state is a metric space with a linear connection with me-tric property. A local homeomorphism between the natural state and the reference state is introduced, say $\mathbf{A}$ in Teodosiu's notation. The linear connection $\mathbf{\Gamma}$ is defined by the formula (19), written for $\mathbf{A}$, which is not a gradient (i.e. an anholonomic tensorial filed). Thus $\mathbf{\Gamma}$ is metric with respect to $\mathbf{C} = \mathbf{A}^T\mathbf{A}$, and Riemann curvature tensor associated with the connection is vanishing.

Generalizing the theory developed by Toupin [28] it is assumed that the stored energy density depends on the the distortion $\mathbf{A}$ and on the specific "covariant" derivative $\nabla_\gamma\mathbf{A}$, which is reformulated by us, under the form

$$\phi = \phi(\mathbf{A}, \mathbf{W}) \tag{27}$$

where $\mathbf{W}$ is the contorsion tensor associated with the connection via Shouten's result.

Comments :

- the variational principle postulated by Toupin is adapted to the considered framework and the stress and hyperstress tensors are derived from the potential defined by the stored energy density, and the balance equations for second grade theory follow, see [15] ;

- the surface gradients of the hypersress enter the boundary conditions ;

- following Kröner's procedure, Teodosiu formulated a generalized scheme for solving the linearized boundary value problems either directly for particular known quasi-dislocation densities, or generally by successive approximations, see [16] and [17].

3.3   Cartan-Riemann geometry of plastically deformed material structure

In the constitutive framework of multiplicative finite elasto-plasticity with second order deformation, developed in the papers Cleja-Ţigoiu [18], Cleja-Ţigoiu et al. [19] we introduced :

Axiom For any motion χ of the body $\mathcal{B}$, at any material particle $\mathbf{X}$ and at any time t, there exists a pair $(\mathbf{F}^p, \overset{(p)}{\mathbf{\Gamma}})$ with $\mathbf{F}^p$ an invertible second order tensor, called plastic distortion and $\overset{(p)}{\mathbf{\Gamma}}_k$ a (1,2) third order field, the so-called called plastic connection. The pair $(\mathbf{F}^p, \overset{(p)}{\mathbf{\Gamma}})$ is invariant with respect to a change of frame in the actual configuration.

Axiom For any pair $(\mathbf{F}, \mathbf{\Gamma})$ of the deformation gradient and motion connection attached to the reference configuration , κ, there exists a *second order pair of elastic deformation*, where the *elastic distorsion* is

defined by

$$\mathbf{F}^e = \mathbf{F}(\mathbf{F}^p)^{-1}, \tag{28}$$

and the *elastic connection* is introduced in terms of the motion and plastic connections, both of them being related to the initial configuration, through the formula

$$\overset{(e)}{\mathbf{\Gamma}}_{\mathcal{K}} = \mathbf{F}^p(\mathbf{\Gamma} - \overset{(p)}{\mathbf{\Gamma}})[(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}]. \tag{29}$$

In the other words we adopted the **composition rule of the second order elastic and plastic deformations**.

We assume that the plastic connection $\overset{(p)}{\mathbf{\Gamma}}$ has metric property with respect to the plastic metric tensor in the reference configuration $\mathbf{C}^p := (\mathbf{F}^p)^T \mathbf{F}^p$.

Let us introduce the Bilby's type connection

$$\overset{(p)}{\mathcal{A}} := (\mathbf{F}^p)^{-1} \nabla \mathbf{F}^p. \tag{30}$$

Proposition. *The plastic connection with metric property with respect to $\mathbf{C}^p$ is represented under the form*

$$\overset{(p)}{\mathbf{\Gamma}} = \overset{(p)}{\mathcal{A}} + (\mathbf{C}^p)^{-1}(\mathbf{\Lambda} \times \mathbf{I}), \tag{31}$$

where the third order tensor $\mathbf{\Lambda} \times \mathbf{I}$, generated by the second order (covariant) tensor $\mathbf{\Lambda}$ is defined by

$$((\mathbf{\Lambda} \times \mathbf{I})\mathbf{u})\mathbf{v} = \mathbf{\Lambda}\mathbf{u} \times \mathbf{v}, \quad \forall \quad \mathbf{u}, \mathbf{v}. \tag{32}$$

$\mathbf{\Lambda}$ is called the disclination tensor.

As a direct consequence of (31) and (30) we get the equivalent representation

$$\mathbf{S}^p = Skw(\overset{(p)}{\mathcal{A}}) + Skw(\mathbf{C}^p)^{-1}(\mathbf{\Lambda} \times \mathbf{I})), \tag{33}$$

Proposition. *The second order torsion tensor $\mathcal{N}^p$ is associated with Cartan torsion and is expressed by*

$$\mathcal{N}^p = (\mathbf{F}^p)^{-1} curl \, \mathbf{F}^p + (\mathbf{C}^p)^{-1}\big((tr \, \mathbf{\Lambda})\mathbf{I} - (\mathbf{\Lambda})^T\big),$$

$$\tag{34}$$

where $\quad (\mathbf{S}^p \mathbf{u})\mathbf{v} = \mathcal{N}^p(\mathbf{u} \times \mathbf{v}).$

Contrary to the elastic models, in the elasto-plastic models at the initial moment we consider that certain heterogeneous distribution of the defects exists inside the material which is considered in a natural state. These defects become active if and only if the elastic stresses, which are determined by solving the elastic problem, reached the appropriate critical values. The defects are characterized by a disclination density tensor, or a dislocation density tensor, respectively. We use arrays of disclination dipoles for modeling the grain boundaries, as they represent the misfit between the lattice orientation of the two single crystalline materials in contact, see [19] and [20].

The basic concepts as balance equations for macro and micro stresses and stress momenta, the principle of free energy imbalance were introduced and developed within continuum mechanics framework.

The free energy density is function of elastic strain and defects, expressed by the torsion tensor associated with the plastic connection, the disclination tensor and its gradient. As for example we assume that the free energy density with respect to the reference configuration is given by a quadratic function with respect to the elastic strain and defects densities, given by

$$\psi = \frac{1}{4}\mathcal{E}(\mathbf{C} - \mathbf{C}^p) \cdot (\mathbf{C} - \mathbf{C}^p) + \frac{1}{2}\beta_2 \mathbf{S}^p \cdot \mathbf{S}^p + \frac{1}{2}\beta_3 \boldsymbol{\Lambda} \cdot \boldsymbol{\Lambda} + \beta_4 \frac{1}{2}\nabla\boldsymbol{\Lambda} \cdot \nabla\boldsymbol{\Lambda}. \tag{35}$$

The parameters involved in the expression of the free energy functions are the components of the elastic stiffness matrix $\mathcal{E}$ and the constant parameters, β_j, j=2,3,4. $\mathcal{E}$ characterizes an orthotrop elastic behaviour.

The *dislocation density tensor*, $\boldsymbol{\alpha}_\mathcal{K}$, is expressed by

$$\boldsymbol{\alpha}_\mathcal{K} := \frac{1}{\det\mathbf{F}^p}(\text{curl }\mathbf{F}^p)(\mathbf{F}^p)^T, \tag{36}$$

and measures the incompatibility of the plastic distortion. The *Burgers vector* associated with the circuit C_0 is defined in terms of the dislocation density.

The *Frank vector* associated with the circuit C_0 is introduced in terms of the disclination tensor, $\widetilde{\boldsymbol{\Lambda}}$, via the disclination density

$$\boldsymbol{\alpha}_\mathcal{K} = \text{curl}(\frac{1}{\det\mathbf{F}^p}\mathbf{F}^p\boldsymbol{\Lambda}) \tag{37}$$

The non-local evolution equations for plastic distortion and disclination tensor were defined to be compatible with the principle of the free energy imbalance. The free energy imbalance formulated in $\mathcal{K}$ and written for any virtual (isothermal) process under the form

$$(\mathcal{P}_{int})_\mathcal{K} - \dot{\psi}_\mathcal{K} \geq 0, \tag{38}$$

see for instance Cleja-Ţigoiu [18]. Here $(\mathcal{P}_{int})_\mathcal{K}$ denotes the internal power expended during the elasto-plastic process and has to be postulated in an appropriate form. $\psi_\mathcal{K}$ is the expression of the free energy function in the configuration $\mathcal{K}$, related to the reference configuration through the plastic distortion.

The complete models for elasto-plastic models with defects such as dislocations, disclinations and grain boundary, as well as the algorithms proposed to simultaneously solve the incremental equilibrium equation, coupled with partial differential equations which describe the defects evolution, can be found in the papers by Cleja-Ţigoiu et al. [19] and [20].

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