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Elasto-viscoplastic Models with Non-Schmid Law and Non-local Evolution of Dislocations in Crystal Lattice

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The paper deals with elasto-plastic materials with crystalline structure, which contain continuously distributed defects as dislocations, within the constitutive framework of second order deformations finite elasto-plasticity. The non-Schmid flow rule describes the evolution of the plastic distortion and the model is dependent on the tensorial measure of dislocation **G** *which is related to the non-zero torsion of plastic connection. A new formula for the time derivative of the* **G** *is derived. The key point to formulate constitutive and evolution laws is the imbalance free energy postulate and the expression of the free energy function. The evolution for the plastic components in the slip systems is described in terms of the generalized stress vector associated with the appropriate Mandel's stress measure, micro momentum defined for plastic mechanism, and gradient of the scalar dislocation densities.*

1 Introduction

The paper deals with elasto-plastic materials with crystalline structure containing continuously distributed defects, with dislocations being considered as possible lattice defects only. If there are defects inside the body, a global stress free configuration does not exist, see Teodosiu (1970), (Mandel, 1972; Cleja-Ţigoiu and Soós, 1990; Cleja-Ţigoiu, 1990a,b). The geometry of the material structure with defects is characterized by the so-called plastic distortion and plastic connection, following (Kondo and Yuki, 1958; Kröner, 1990, 1992). Our model is developed within the constitutive framework of finite elasto-plasticity based on the decomposition of the second order deformation associated with the body motion into elastic and plastic second order deformations, its rationale being set by Cross (1973) and Wang (1973). The multiplicative decomposition of the deformation gradient and the transformation rule of the connections are introduced following (Cleja-Ţigoiu, 2007, 2010). We postulate that the plastic connection has non-zero Cartan torsion. The Cartan torsion is viewed as a tensorial measure of dislocations, which is sometimes called *the defect density tensor*, or *geometrically necessary dislocations*. On the background of the differential geometry concepts the continuously distributed dislocations are modeled by (Teodosiu, 1970; Steinmann, 1996; Forest et al., 1997; Cleja-Ţigoiu, 2002; Clayton et al., 2006) starting from (Bilby, 1960; Kondo and Yuki, 1958; de Wit, 1981). The differential geometry concepts in terms of component representations in classical tensor analysis can be found in (Schouten, 1954; Clayton et al., 2006; Kröner, 1990, 1992) as well as in (Noll, 1974; Epstein, 2010). Our model is developed within the constitutive framework of continuum mechanics in the formalism proposed by Truesdell and Noll (1965). No Cosserat type kinematics and no micromorphic effects have been assumed in the model. Various decompositions of the strain gradient of the displacement in the elastoviscoplastic generalized continua were proposed and developed by Forest and Sievert (2003).

The constitutive framework is compatible with the free energy imbalance principle, formulated by (Cleja-Ţigoiu, 2007, 2010), following (Gurtin, 2000, 2004; Gurtin et al., 2010). The constitutive description is first described with respect to the crystal configuration.

The key point is the form of the postulate of the imbalance of the free energy related to the expression of the internal dissipated power, as well as the free energy function, see the methodology developed in (Gurtin, 2000, 2004; Gurtin et al., 2010), and Cleja-Ţigoiu (2007, 2010) for second order elasto-plasticity. Within the constitutive framework proposed in Cleja-Ţigoiu (2013), the micro momentum related to the plastic mechanism, and the micro forces related to the dislocation mechanism produce internal power.

Here we start from the assumption that the non-Schmid flow rule describes the evolution of the plastic distortion, as Kuroda (2003); Dao and Asaro (1996); Cleja-Ţigoiu and Paşcan (2013a) considered. The plastic compressibility effect has been introduced here via the normal components of the rate of plastic distortion and associated with the normal to the crystallographic systems, apart from the model proposed by Aslan et al. (2011). In the aforementioned paper this effect is considered to be generated by the damage, which is coupled to the irreversible behaviour and is defined in terms of the normal vectors to the crystallographic damage planes. In the model proposed here the rate of plastic distortion involves not only the shear rates but the normal velocities in the slip systems. These scalar velocities are time derivatives of certain scalar fields, which are generically called the *plastic scalar components* in the slip systems associated with the lattice structure. The novelty herein consists in the presence of the Cartan torsion, when the influence of the disclination tensor $\boldsymbol{\Lambda}$ is not considered, namely through $\mathbf{G}$ -(GND) dislocation tensor. The new formula gives rise to the time derivative of $\mathbf{G}$ in terms of the gradients of plastic velocity components. The free energy density function is assumed to be dependent on the elastic strain, on the plastic scalar components in the slip systems associated with the lattice structure and their gradients, as well as on the scalar dislocation density (the so called statistically stored dislocations) and their gradient. The gradients of the plastic scalar components prove enter the circumstantial dependence of the free energy density function on the tensorial dislocation density.

Our goal is to derive the non-local evolution equations for the components of plastic distortion and the scalar dislocation densities, which are compatible with the imbalance of the free energy density. We analyze the constitutive restrictions resulting from the assumption that the non-Schmid law occurs and compare our results with those earlier obtained in the paper by Cleja-Ţigoiu and Paşcan (2013b), (Gurtin, 2000, 2004), when we restricted ourselves to multislip flow rule, as in finite deformation crystal plasticity.

1.1 List of Notations and Definitions

The following notations and definition will be used in the further calculations:

$\mathbf{u}\cdot\mathbf{v}, \mathbf{u}\times\mathbf{v}, \mathbf{u}\otimes\mathbf{v}$ denote scalar, cross and tensorial products of vectors;
$\mathbf{a}\otimes\mathbf{b}$ and $\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c}$ are defined to be a second order tensor and a third order tensor by
$(\mathbf{a}\otimes\mathbf{b})\mathbf{u}=\mathbf{a}(\mathbf{b}\cdot\mathbf{u}), \quad (\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c})\mathbf{u}=(\mathbf{a}\otimes\mathbf{b})(\mathbf{c}\cdot\mathbf{u}),$ for all vectors $\mathbf{u}\in\mathcal{V}$.
For $\mathbf{A}\in Lin -$ a second order tensor, we introduce:
the notations $\{\mathbf{A}\}^S, \{\mathbf{A}\}^a$ for the symmetric and skew-symmetric parts of the tensor;
the tensorial product $\mathbf{A}\otimes\mathbf{a}$ for $\mathbf{a}\in\mathcal{V}$, is a third order tensor, with the property
$(\mathbf{A}\otimes\mathbf{a})\mathbf{v}=\mathbf{A}(\mathbf{a}\cdot\mathbf{v}), \quad \mathbf{A}\cdot(\mathbf{a}\otimes\mathbf{v})=\mathbf{a}\cdot(\mathbf{A}\mathbf{v}), \forall\mathbf{v}\in\mathcal{V}.$

I is the identity tensor in Lin, $\mathbf{A}^T$ denotes the transpose of $\mathbf{A}\in Lin$,

$\nabla\mathbf{A}$ is the derivative (or the gradient) of the field $\mathbf{A}$ in a coordinate system $\{\mathbf{x}^a\}$ (with respect to the reference configuration), $\nabla\mathbf{A} = \dfrac{\partial A_{ij}}{\partial x^k}\mathbf{e}^i\otimes\mathbf{e}^j\otimes\mathbf{e}^k$. The coordinate basis vector corresponding to $\mathbf{x}^a$ are denoted by $\mathbf{e}_a$, while the dual basis $\mathbf{e}^a$, is defined by the inner product $\mathbf{e}^b\cdot\mathbf{e}_a = \delta^b{}_a$.

Definition of the curl:

$$(\text{curl}\mathbf{A})(\mathbf{u}\times\mathbf{v}) = ((\nabla\mathbf{A})\mathbf{u})\mathbf{v} - ((\nabla\mathbf{A})\mathbf{v})\mathbf{u}, \quad \forall \quad \text{vectors} \quad \mathbf{u},\mathbf{v},\mathbf{z}\in\mathcal{V}; \tag{1}$$

$Lin(\mathcal{V}, Lin) = \{\mathbf{N} : \mathcal{V} \longrightarrow Lin, \quad \text{linear}\}-$ defines the space of all third order tensors and it is given by **N** = $N_{ijk}\mathbf{i}^i\otimes\mathbf{i}^j\otimes\mathbf{i}^k$.

The scalar product of two second order tensor $\mathbf{A},\mathbf{B}$ is $\mathbf{A}\cdot\mathbf{B} := \text{tr}(\mathbf{A}\mathbf{B}^T) = A_{ij}B_{ij},$ and the scalar product of third order tensors is given by $\mathbf{N}\cdot\mathbf{M} = N_{ijk}M_{ijk},$ in a Cartesian system coordinate, and $\mathbf{A}\cdot\mathbf{B} = A_{ab}B^{ab}$ in a local coordinate system.

The product ":" of a second order tensor $\mathbf{A}$ and a third order tensor $\mathbf{M}$ is a vector, which is defined by $\mathbf{A} : \mathbf{M}$

$$(\mathbf{A} : \mathbf{M})\cdot\mathbf{u} = \mathbf{A}\cdot(\mathbf{M}\mathbf{u}), \text{ for all } \mathbf{u}\in\mathcal{V} \tag{2}$$

We make the difference between the gradient in local coordinate and the covariant derivative for a vector field, say $\mathbf{Y}$,

$$\nabla\mathbf{Y} = \frac{\partial Y^a}{\partial x^b}\mathbf{e}_a\otimes\mathbf{e}^b, \quad \nabla_{\boldsymbol{\Gamma}}\mathbf{Y} = (\frac{\partial Y^a}{\partial x^b} + Y^c\Gamma^a_{cb})\mathbf{e}_a\otimes\mathbf{e}^b$$

and for a second order tensor field, respectively, say for $\mathbf{C}$,

$$\nabla \mathbf{C} = \frac{\partial C_{lm}}{\partial x^k} \mathbf{e}^l \otimes \mathbf{e}^m \otimes \mathbf{e}^k,$$
$$\nabla_{\mathbf{\Gamma}} \mathbf{C} = (\frac{\partial C_{lm}}{\partial x^k} - \Gamma^i_{lk} C_{im} - C_{li} \Gamma^i_{mk})(\mathbf{e}^l \otimes \mathbf{e}^m \otimes \mathbf{e}^k). \tag{3}$$

The covariant derivatives are calculated with respect to a given affine connection, defined in a coordinate system by

$$\mathbf{\Gamma} = \Gamma^i_{mk} \mathbf{e}_i \otimes \mathbf{e}^m \otimes \mathbf{e}^k. \tag{4}$$

We introduce a third order tensor field generated by a third order field, say $\mathcal{A}$, together with the second order tensors, for instance $\mathbf{F}_1, \mathbf{F}_2$:

$$(\mathcal{A}[\mathbf{F}_1, \mathbf{F}_2]\mathbf{u})\mathbf{v} = (\mathcal{A}(\mathbf{F}_1 \mathbf{u}))\, \mathbf{F}_2 \mathbf{v}, \quad \forall \mathbf{u}, \mathbf{v} \in \mathcal{V}. \tag{5}$$

The following calculus rules yield for $\mathbf{F}_j \in Lin$ and $\mathcal{A}, \mathcal{B}$, third order tensors,

$$\mathcal{A} \cdot \mathcal{B}\mathbf{F}_1 = \mathcal{A}\mathbf{F}_1^T \cdot \mathcal{B}$$
$$(\mathcal{A}[\mathbf{F}_1, \mathbf{F}_2])[\mathbf{F}_3, \mathbf{F}_4] = (\mathcal{A}[\mathbf{F}_1\mathbf{F}_3,\ \mathbf{F}_2\mathbf{F}_4] \tag{6}$$

For any $\mathbf{\Lambda}_1$, $\mathbf{\Lambda}_2 \in Lin$ we define a third order tensor associated with them, denoted $\mathbf{\Lambda_1} \times \mathbf{\Lambda}_2$, by

$$((\mathbf{\Lambda}_1 \times \mathbf{\Lambda}_2)\mathbf{u})\mathbf{v} = (\mathbf{\Lambda}_1 \mathbf{u}) \times (\mathbf{\Lambda}_2 \mathbf{v}), \quad \forall \quad \mathbf{u}, \mathbf{v}. \tag{7}$$

$\tilde{\rho}, \hat{\rho}, \hat{\rho}_0$ are the mass densities with respect to the lattice state, current and reference configurations.

2 Constitutive Framework

If there are defects inside the body, a global stress free configuration does not exist (see (Mandel, 1972; Teodosiu, 1970; Cleja-Ţigoiu and Soós, 1990)) and the geometry of the material structure with defects is characterized by the so-called plastic distortion, $\mathbf{F}^p$, and plastic connection, $\overset{(\mathrm{p})}{\mathbf{\Gamma}}$.

In this paper three configurations will be considered:

• k a fixed reference configuration of the body $\mathcal{B}$, $k(\mathcal{B}) \subset \mathcal{E}-$ the Euclidean space, with the vector space $\mathcal{V}$;

• $\chi(\cdot, t)$ the deformed configuration at time t, where $\chi : \mathcal{B} \times R \to \mathcal{E}$ defines the motion of the body $\mathcal{B}$, R being the set of real numbers;

• the isoclinic (anholonomic) configuration related to the lattice structure, denoted $\mathcal{K}$.

2.1 Geometric and Kinematic Relationships

Ax. 1 The plastic connection has metric property which is formalized by the following relationship

$$(\nabla\ \mathbf{C}^p)\mathbf{u} = \mathbf{C}^p \overset{(\mathrm{p})}{\mathbf{\Gamma}}\ \mathbf{u} + (\mathbf{C}^p\ \ \overset{(\mathrm{p})}{\mathbf{\Gamma}}\ \mathbf{u})^T, \quad \mathbf{C}^p = (\mathbf{F}^p)^T \mathbf{F}^p, \tag{8}$$

$\mathbf{C}^p$ represents the *plastic metric tensor*. In Cleja-Ţigoiu (2007) it is proved that

Theorem 1. *The plastic connection (in a coordinate system) with metric property with respect to* $\mathbf{C}^p$ *is represented* *by*

$$\overset{(p)}{\mathbf{\Gamma}} = (\mathbf{C}^p)^{-1}(\overset{(p)}{\mathcal{A}} + \mathbf{\Lambda}\times\mathbf{I}), \quad \textit{where} \quad \overset{(p)}{\mathcal{A}} := (\mathbf{F}^p)^{-1}\nabla\mathbf{F}^p \tag{9}$$

is Bilby's type connection and $\mathbf{\Lambda}$ denotes the disclination (second order) tensor.

The *Cartan torsion* associated with the plastic connection, $\mathbf{S}^p$, as a third order tensor is given by

$$(\mathbf{S}^p\mathbf{u})\mathbf{v} = (\overset{(p)}{\mathbf{\Gamma}}\ \mathbf{u})\mathbf{v} - (\overset{(p)}{\mathbf{\Gamma}}\ \mathbf{v})\mathbf{u}$$

and the *second order torsion tensor*, $\mathcal{N}^p$, is expressed by

$$(\mathbf{S}^p\mathbf{u})\mathbf{v} = \mathcal{N}^p(\mathbf{u}\times\mathbf{v}), \tag{10}$$

for all vectors $\mathbf{u}$ and $\mathbf{v}$. **Theorem 2.** *The second order torsion tensor $\mathcal{N}^p$, associated with the Cartan torsion, is expressed by*

$$\mathcal{N}^p = (\mathbf{F}^p)^{-1}\textit{curl}\mathbf{F}^p + (\mathbf{C}^p)^{-1}\big((\textit{tr}\ \mathbf{\Lambda})\mathbf{I} - (\mathbf{\Lambda})^T\big). \tag{11}$$

The following defect fields (as second order fields) have been introduced of the Cartan tensor $\mathcal{N}^p$

$$\begin{aligned} \boldsymbol{\alpha} \quad & := (\mathbf{F}^p)^{-1}\text{curl}(\mathbf{F}^p), \\ & \text{which is called the Noll dislocation densityNoll (1974)} \\ \boldsymbol{\alpha}^{\Lambda} \quad & := \text{tr }\mathbf{\Lambda}\mathbf{I} - (\mathbf{\Lambda})^T, \\ & \boldsymbol{\alpha}^{\Lambda} \text{ is called the disclination density.} \end{aligned} \tag{12}$$

They characterize *incompatibilities* existing in the materials, , see de Wit (1981).

Let $\mathbf{F}(\mathbf{X},t) = \nabla\chi(\mathbf{X},t)$ be the deformation gradient at time t, for any $\mathbf{X}\in\mathcal{B}$, and $\mathbf{\Gamma} = \mathbf{F}^{-1}\nabla\mathbf{F}$ be the motion connection or the material connection.

Ax. 2 The decomposition of the second order deformation, $(\mathbf{F},\mathbf{\Gamma})$, associated with the motion of the body $\mathcal{B}$, into elastic and plastic second order deformations is assumed to be given by

$$\begin{aligned} &\mathbf{F} = \mathbf{F}^e\mathbf{F}^p, \\ &\mathbf{\Gamma} = \overset{(p)}{\mathbf{\Gamma}} + (\mathbf{F}^p)^{-1}\ \overset{(e)}{\mathbf{\Gamma}}_{\mathcal{K}}\ [\mathbf{F}^p,\mathbf{F}^p], \quad \mathbf{\Gamma} = \mathbf{F}^{-1}\nabla\mathbf{F}. \end{aligned} \tag{13}$$

We remark that there exists an *anholonomic configuration*, $\mathcal{K}$, which is associated with the second order plastic deformation, namely $(\mathbf{F}^p, \overset{(p)}{\mathbf{\Gamma}})$.

The following calculus laws hold:

a. The gradient in the configuration $\mathcal{K}$ of the field $\mathbf{F}$, $\nabla_{\mathcal{K}}\mathbf{F}$, is calculated by

$$\nabla_{\mathcal{K}}\mathbf{F} := (\nabla\mathbf{F})(\mathbf{F}^p)^{-1}, \tag{14}$$

$\nabla\mathbf{F}$ is a gradient in the reference configuration.

b. The plastic connection with respect to the anholonomic configuration, $\mathcal{K}$, denoted by $\overset{(p)}{\mathbf{\Gamma}}_{\mathcal{K}}$, is related to the plastic connection, $\overset{(p)}{\mathbf{\Gamma}}$, previously defined with respect to the reference configuration, by the following relationship

$$\overset{(p)}{\mathbf{\Gamma}}_{\mathcal{K}} = -\mathbf{F}^p\ \overset{(p)}{\mathbf{\Gamma}}\ [(\mathbf{F}^p)^{-1},(\mathbf{F}^p)^{-1}]. \tag{15}$$

As a direct consequence of the multiplicative decomposition of the deformation gradient into its components, $(13)_1$, 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

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e\,\mathbf{L}^p\,\left(\mathbf{F}^e\right)^{-1}, \quad \mathbf{L}^e = \dot{\mathbf{F}}^e\,\left(\mathbf{F}^e\right)^{-1}, \quad \mathbf{L}^p = \dot{\mathbf{F}}^p\,\left(\mathbf{F}^p\right)^{-1}. \tag{16}$$

2.2 Model with Non-Schmid Plastic Evolution Law

Ax. 3 The evolution equation for the plastic distortion is given by a non-Schmid's law, that involves not only the plastic shear rates in the slip system, but also the normal velocity to the slip system

$$\dot{\mathbf{F}}^p\,\left(\mathbf{F}^p\right)^{-1} = \sum_{\alpha=1}^{N} \nu^\alpha\,(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) + \sum_{\alpha=1}^{N} \hat{\nu}^\alpha\,(\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha) + \tilde{\nu}\,\mathbf{I}, \tag{17}$$

where N is the number of slip-systems, ν^α is the slip velocity, $\hat{\nu}^\alpha$ is the normal velocity on the $\alpha-$slip system, $\tilde{\nu}$ characterizes the rate of plastic volume expansion.

Denote by $(\mathbf{s}^\alpha, \mathbf{m}^\alpha)$ the $\alpha-$slip system in the lattice configuration, where $\mathbf{m}^\alpha$ is the normal to the slip plane, $\mathbf{s}^\alpha$ is the slip direction and $\mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0$.

The $\alpha-$ slip system pulled back to the reference configuration is characterized by the vectors $(\hat{\mathbf{s}}^\alpha, \hat{\mathbf{m}}^\alpha)$,

$$\hat{\mathbf{m}}^\alpha = (\mathbf{F}^p)^T \mathbf{m}^\alpha, \quad \hat{\mathbf{s}}^\alpha = (\mathbf{F}^p)^{-1} \mathbf{s}^\alpha, \tag{18}$$

which remain orthogonal.

Let us introduce the rate of plastic distorsion with respect to the reference configuration, $\hat{\mathbf{l}}^p$, and its representation

$$\begin{aligned} &\hat{\mathbf{l}}^p := (\mathbf{F}^p)^{-1}\dot{\mathbf{F}}^p = (\mathbf{F}^p)^{-1}\,\mathbf{L}^p\,\mathbf{F}^p, \\ &\hat{\mathbf{l}}^p = \sum_{\alpha=1}^{N} \nu^\alpha\,(\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) + \sum_{\alpha=1}^{N} \hat{\nu}^\alpha\,\left(\mathbf{C}^p\right)^{-1}(\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha)\,\right) + \tilde{\nu}\,\mathbf{I}. \end{aligned} \tag{19}$$

As a consequence of the definition for the Bilby type plastic connection, and the hypothesis concerning the expression of the rate of plastic distorsion (17), one obtains the time derivative of $(9)_2$

$$\begin{aligned} \frac{d}{dt}(\overset{(\mathrm{p})}{\mathcal{A}}) &= \sum_{\alpha=1}^{N} (\mathbf{F}^p)^{-1}\{\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \otimes \nabla\nu^\alpha\}[\mathbf{I}, \mathbf{F}^p] + \\ &+ \sum_{\alpha=1}^{N} (\mathbf{F}^p)^{-1}\{\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha \otimes \nabla\hat{\nu}^\alpha\}[\mathbf{I}, \mathbf{F}^p] + (\mathbf{I} \otimes \nabla\tilde{\nu}). \end{aligned} \tag{20}$$

Let us introduce our definition for (GND) dislocation density tensor

$$\begin{aligned} &\mathbf{G} \equiv \boldsymbol{\alpha} = (\mathbf{F}^p)^{-1}\mathrm{curl}\mathbf{F}^p, \text{or its equivalent expression} \\ &\mathbf{G}(\mathbf{u} \times \mathbf{v}) = (\overset{(\mathrm{p})}{\mathcal{A}}\,\mathbf{u})\mathbf{v} - (\overset{(\mathrm{p})}{\mathcal{A}}\,\mathbf{v})\mathbf{u}, \end{aligned} \tag{21}$$

that holds for any vector fields $\mathbf{u}, \mathbf{v}$. In order to compute the time derivative of (GND)- dislocation density we start from the relationship

$$(\frac{d}{dt}\mathbf{G})(\mathbf{u} \times \mathbf{v}) = ((\frac{d}{dt}\,\overset{(\mathrm{p})}{\mathcal{A}})\mathbf{u})\mathbf{v} - (\frac{d}{dt}\,\overset{(\mathrm{p})}{\mathcal{A}}\,\mathbf{v})\mathbf{u}, \tag{22}$$

written for all $\mathbf{u}$ and $\mathbf{v}$.

As a consequence of the definitions and the properties introduced above the derivative with respect to time for **G** can be expressed by

Theorem 3.

$$
\begin{aligned}
\frac{d}{dt}\mathbf{G} \;&= \sum_{\alpha=1}^{N} \frac{1}{\mid \hat{\mathbf{s}}^{\alpha} \mid^2} (\nabla \nu^{\alpha} \cdot \hat{\mathbf{s}}^{\alpha}) \hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{p}}^{\alpha} - \sum_{\alpha=1}^{N} \frac{1}{\mid \hat{\mathbf{s}}^{\alpha} \mid^2} (\nabla \nu^{\alpha} \cdot \hat{\mathbf{p}}^{\alpha}) \hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{s}}^{\alpha} + \\
&+ (\mathbf{C})^{-1} \sum_{\alpha=1}^{N} \frac{1}{\mid \hat{\mathbf{s}}^{\alpha} \mid^2} \big((\nabla \hat{\nu}^{\alpha} \cdot \hat{\mathbf{s}}^{\alpha}) \hat{\mathbf{m}}^{\alpha} \otimes \hat{\mathbf{p}}^{\alpha} - (\nabla \hat{\nu}^{\alpha} \cdot \hat{\mathbf{p}}^{\alpha}) \hat{\mathbf{m}}^{\alpha} \otimes \hat{\mathbf{s}}^{\alpha} \big) + \in \nabla \tilde{\nu}, \\
&\textit{where} \quad \hat{\mathbf{p}}^{\alpha} = \hat{\mathbf{s}}^{\alpha} \times \hat{\mathbf{m}}^{\alpha}, \quad \mid \hat{\mathbf{s}}^{\alpha} \mid^2 = \mathbf{s}^{\alpha} \cdot \mathbf{c}^{p} \mathbf{s}^{\alpha}, \quad \mathbf{c}^{p} = (\mathbf{F}^{p})^{-T} (\mathbf{F}^{p})^{-1}.
\end{aligned}
\tag{23}
$$

Here $\in$ *is a permutation symbol which is introduced via the equality*

$$((\mathbf{I} \otimes \nabla \tilde{\nu})\mathbf{u})\mathbf{v} - ((\mathbf{I} \otimes \nabla \tilde{\nu})\mathbf{v})\mathbf{u} = \in \nabla \tilde{\nu} (\mathbf{u} \times \mathbf{v}). \tag{24}$$

The hat-vectors define an orthogonal basis by the following relationships

$$
\begin{aligned}
&\hat{\mathbf{p}}^{\alpha} = \hat{\mathbf{s}}^{\alpha} \times \hat{\mathbf{m}}^{\alpha}, \quad \mid \hat{\mathbf{p}}^{\alpha} \mid = \mid \hat{\mathbf{s}}^{\alpha} \mid\mid \hat{\mathbf{m}}^{\alpha} \mid \\
&\hat{\mathbf{s}}^{\alpha} = \frac{1}{\mid \hat{\mathbf{m}}^{\alpha} \mid^2} \hat{\mathbf{m}}^{\alpha} \times \hat{\mathbf{p}}^{\alpha}, \quad \mid \hat{\mathbf{m}}^{\alpha} \mid^2 = \mathbf{m}^{\alpha} \cdot \mathbf{B}^{p} \mathbf{m}^{\alpha}, \quad \mathbf{B}^{p} = \mathbf{F}^{p} (\mathbf{F}^{p})^{T}.
\end{aligned}
\tag{25}
$$

We sketch the **proof.** Let us introduce the third order tensor $Skw\mathcal{A}^{p}$, which is associated with $\mathcal{A}^{p}$ by the formula

$$((Skw\mathcal{A}^{p})\mathbf{u})\mathbf{v} = (\mathcal{A}^{p}\mathbf{u})\mathbf{v} - (\mathcal{A}^{p}\mathbf{v})\mathbf{u}, \tag{26}$$

written for all $\mathbf{u}, \mathbf{v}$.

The gradient of the plastic velocity component, say of $\nabla \nu^{\alpha}$, is projected on the orthogonal basis $(\hat{\mathbf{s}}^{\alpha}, \hat{\mathbf{m}}^{\alpha}, \hat{\mathbf{p}}^{\alpha})$ and the following formula holds

$$\nabla \nu^{\alpha} = \frac{1}{\mid \hat{\mathbf{m}}^{\alpha} \mid^2} (\nabla \nu^{\alpha} \cdot \hat{\mathbf{m}}^{\alpha})\, \hat{\mathbf{m}}^{\alpha} + \frac{1}{\mid \hat{\mathbf{s}}^{\alpha} \mid^2} (\nabla \nu^{\alpha} \cdot \hat{\mathbf{s}}^{\alpha})\, \hat{\mathbf{s}}^{\alpha} + \frac{1}{\mid \hat{\mathbf{p}}^{\alpha} \mid^2} (\nabla \nu^{\alpha} \cdot \hat{\mathbf{p}}^{\alpha})\, \hat{\mathbf{p}}^{\alpha}. \tag{27}$$

We calculate the derivative $Skw(\frac{d}{dt}(\overset{(\mathrm{p})}{\mathcal{A}}))$. We arrive at the evaluation of the differences of the form

$$
\begin{aligned}
&((\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha})\mathbf{u})\mathbf{v} - ((\hat{\mathbf{s}}^{\alpha} \otimes \hat{\mathbf{m}}^{\alpha})\mathbf{v})\mathbf{u} = \mathbf{\Omega} \cdot (\mathbf{u} \times \mathbf{v}), \\
&\text{where } \mathbf{\Omega} = -\hat{\mathbf{s}}^{\alpha} \times \hat{\mathbf{m}}^{\alpha}.
\end{aligned}
\tag{28}
$$

$\mathbf{\Omega}$ is the coaxial vector, associate with the appropriate skew-symmetric tensor.

Comment 1: The rate of the tensorial dislocation filed **G** contains $\nabla \nu^{\alpha}, \nabla \hat{\nu}^{\alpha}, \nabla \tilde{\nu}$, which are time derivatives of plastic components gradients in slip system. These fields $\nabla \gamma^{\alpha}, \nabla \hat{\gamma}^{\alpha}, \nabla \tilde{\gamma}$ enter the expression of the free energy density and prove the circumstantial dependence on the tensorial dislocation density.

Comment 2: We emphasized the expression for the time derivative of GND-density tensor, with respect to the slip system pulled back to the reference configuration. We can compare (23) with other results in literature, only with regards to the Schmid effect (i.e. when the normal plastic components $\hat{\gamma}^{\alpha}, \tilde{\gamma}$ do not appear) in (23). The definition of the lattice tensor field $\mathbf{G}^{C} = \mathbf{F}^{p}\mathrm{curl}\mathbf{F}^{p}$, (the so-called geometrically necessary dislocation tensor), has been introduced by Cermelli and Gurtin (2001, 2002). Here we denoted this tensor by $\mathbf{G}^{C}$ to make difference between them. The plastically convected rate of $\mathbf{G}^{C}$ has a similar expression as in (23), when $\hat{\mathbf{m}}$ is absent. The rate of macroscopic distribution of screw and edge dislocations were introduced in Cermelli and Gurtin (2001, 2002) as the coefficients of the appropriate tensorial products. Another formula for scalar dislocation densities associated with a GND- density tensor has been introduced by Mayeur et al. (2011).

3 Model with Scalar and Tensorial Dislocation Densities

Within the constitutive framework of finite elasto-plasticity with second order deformation, the paper by Cleja-Ţigoiu (2013) proposes the models with

- *tensorial measure of the dislocation*: $\overset{(\mathrm{p})}{\mathcal{A}} = (\mathbf{F}^p)^{-1}(\nabla\ \mathbf{F}^p)$, and
- scalar dislocation density, say ρ^d.

Only the skew-symmetric part of $\overset{(\mathrm{p})}{\mathcal{A}}$ enters the definition of the tensorial measure of dislocation density.

In the presented here model, we introduce the non-Schmid plastic law and we analyze the resulting consequences on the constitutive and evolution equations which are compatible with the free energy imbalance principle.

Let us introduce the scalar dislocation density with respect to the lattice configuration $\rho^d_{\mathcal{K}}$ and its gradient

$$\begin{aligned} &\rho^d_{\mathcal{K}} = \frac{1}{J^p}\rho^d \\ &\nabla_{\mathcal{K}}\rho^d_{\mathcal{K}} := \frac{1}{J^p}(\mathbf{F}^p)^{-T}\nabla\rho^d, \quad J^p = \mid \det\mathbf{F}^p \mid \end{aligned} \tag{29}$$

The time derivatives of the scalar dislocation density and its gradient have the following expressions

$$\begin{aligned} &\frac{d}{dt}\rho^d_{\mathcal{K}} = \frac{1}{J^p}(\dot{\rho}^d - \rho^d \ \mathrm{tr}\mathbf{L}^p), \\ &J^p\ \frac{d}{dt}(\nabla_{\mathcal{K}}(\rho^d_{\mathcal{K}})) = -\mathrm{tr}\ \mathbf{L}^p(\mathbf{F}^p)^{-T}\nabla\rho^d - ((\mathbf{F}^p)^{-1}\mathbf{L}^p)^T\ \nabla\rho^d + (\mathbf{F}^p)^{-T}\nabla\dot{\rho}^d. \end{aligned} \tag{30}$$

Ax. 3 (Free energy imbalance in the lattice space)

The material behavior is restricted to satisfy in $\mathcal{K}$ the *free energy imbalance postulate*, which states that the time derivative of the free energy density can not be grater or equal than the internal power

$$-\dot{\psi}_{\mathcal{K}} + (\mathcal{P}_{int})_{\mathcal{K}} \geq 0 \tag{31}$$

We assume here:

- the free energy density with respect to the lattice configuration is given as a function dependent on the set of variables written in the reference configuration, namely

  $$\psi = \psi_{\mathcal{K}} \equiv \psi(\mathbf{C}-\mathbf{C}^p, \gamma^\alpha, \hat{\gamma}^\alpha, \tilde{\gamma}, \nabla\gamma^\alpha, \nabla\hat{\gamma}^\alpha, \nabla\tilde{\gamma}, \rho^d, \nabla\rho^d), \quad \mathbf{C} = (\mathbf{F})^T\mathbf{F}. \tag{32}$$

  $\mathbf{C}^e - \mathbf{I} = (\mathbf{F}^p)^{-T}(\mathbf{C}-\mathbf{C}^p)(\mathbf{F}^p)^{-1}$. The presence of the plastic distortion, $\mathbf{F}^p$, and its gradient through $\overset{(\mathrm{p})}{\mathcal{A}}$, is generically represented by $\mathbf{C}-\mathbf{C}^p$, the scalar plastic components and their gradients, see comment 1. The free energy density depends on the scalar dislocation density and its gradient;
- an appropriate definition for the internal power $(\mathcal{P}_{int})_{\mathcal{K}}$, extended to involve the expound power resulting from forces conjugated with the appropriate rate of elastic and plastic second order deformations, as well as the power dissipated in the dislocation mechanism is proposed;
- the free energy imbalance is postulated for any virtual (isothermic) processes, associated with *kinematics* of the deformation process.

If the free energy density is dependent on the second order elastic deformation only through the elastic strain, $\mathbf{C}^e = (\mathbf{F}^e)^T\mathbf{F}^e$, namely it is not dependent on the Bilby type elastic connection, then the macro stress momentum vanishes, see Cleja-Ţigoiu (2010). The *balance equation* for macro stress and macro momentum (Cleja-Ţigoiu, 2007; Fleck et al., 1994) is reduced to the classical one. As it is the case considered here, we do not include the macro momentum in the expression of the internal power.

Ax. 4 The internal power in the lattice space is given by the expression

$$
\begin{aligned}
(\mathcal{P}_{int})_{\mathcal{K}} \quad &= \frac{1}{2\widetilde{\rho}}\,\boldsymbol{\pi}\cdot\dot{\mathbf{C}}^e + \frac{1}{\widetilde{\rho}}\mathbf{g}^p\cdot\mathbf{L}^p + \frac{1}{\widetilde{\rho}}\boldsymbol{\mu}^p\cdot\nabla_{\mathcal{K}}\mathbf{L}^p + \\
&+\frac{1}{\widetilde{\rho}}g^d\cdot\frac{d}{dt}(\rho^d_{\mathcal{K}}) + \frac{1}{\widetilde{\rho}}\boldsymbol{\mu}^d\cdot\frac{d}{dt}(\nabla_{\mathcal{K}}{\rho^d}_{\mathcal{K}}).
\end{aligned}
\tag{33}
$$

- $\boldsymbol{\pi}$ is the Piola-Kirchhoff stress tensor related to the Cauchy stress tensor $\mathbf{T}$ by $\boldsymbol{\pi} = \det\mathbf{F}^e(\mathbf{F}^e)^{-1}\mathbf{T}(\mathbf{F}^e)^{-T}$.
- The micro forces $(\mathbf{g}^p, \boldsymbol{\mu}^p)$ are related to the plastic deformation mechanism, they are power conjugated with the plastic rate and its gradient in lattice space, $(\mathbf{L}^p, \nabla_{\mathcal{K}}\mathbf{L}^p)$, and satisfy the micro balance equation in $\mathcal{K}$

$$
\mathbf{g}^p = \mathrm{div}_{\mathcal{K}}\,(\boldsymbol{\mu}^p) + \tilde{\rho}\mathbf{B}^p_m. \tag{34}
$$

$\mathbf{B}^p_m$ mass density of the couple body force, see Cleja-Ţigoiu (2013).

Proposition 1. The micro balance equation (34) is equivalently written with respect to the reference configuration

$$
J^p\;\mathbf{g}^p = \mathrm{div}\,(J^p\boldsymbol{\mu}^p(\mathbf{F}^p)^{-1}) + \hat{\rho}\mathbf{B}^p_m. \tag{35}
$$

$\mathbf{B}^p_m$ mass density of the couple body force.

- The dissipated power produced by the micro stress related with plastic mechanism is given

$$
\frac{1}{\tilde{\rho}}\mathbf{g}^p\cdot\mathbf{L}^p = \frac{1}{\rho_0}\boldsymbol{\Sigma}^p_0\cdot\hat{\mathbf{l}}^p, \quad \text{with} \quad \frac{1}{\hat{\rho}_0}\boldsymbol{\Sigma}^p_0 = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^T\mathbf{g}^p(\mathbf{F}^p)^{-T}. \tag{36}
$$

Here $\boldsymbol{\Sigma}^p_0$ is the Mandel's stress measure associated with the micro plastic stress $\mathbf{g}^p$.

As a consequence of the definition $(19)_1$ and the formula (36) the power delivered by $\mathbf{g}^p$ is given by

$$
\sum_{\alpha=1}^{N}\frac{1}{\rho_0}\boldsymbol{\Sigma}^p_0\cdot\;(\hat{\mathbf{s}}^\alpha\otimes\hat{\mathbf{m}}^\alpha)\,\nu^\alpha + \sum_{\alpha=1}^{N}\;\frac{1}{\rho_0}\boldsymbol{\Sigma}^p_0\cdot((\mathbf{C}^p)^{-1}\hat{\mathbf{m}}^\alpha\otimes\hat{\mathbf{m}}^\alpha)\,\hat{\nu}^\alpha + \tilde{\nu}\,\frac{1}{\rho_0}\boldsymbol{\Sigma}^p_0\cdot\mathbf{I} \tag{37}
$$

In order to express the power expanded by the plastic micro momentum we proceed as follows

- First we recall the formula which gives the gradient, $\nabla_{\mathcal{K}}\mathbf{L}^p$, second we replace the time derivative of $\overset{(\mathrm{p})}{\mathcal{A}}$ through the expression (20), and finally it results

$$
\begin{aligned}
\nabla_{\mathcal{K}}\mathbf{L}^p &= \mathbf{F}^p\frac{d}{dt}(\overset{(\mathrm{p})}{\mathcal{A}})[(\mathbf{F}^p)^{-1},(\mathbf{F}^p)^{-1}] = \sum_{\alpha=1}^{N}\{\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\nu^\alpha\}[(\mathbf{F}^p)^{-1},\mathbf{I}] + \\
&+\sum_{\alpha=1}^{N}\{\mathbf{m}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\hat{\nu}^\alpha\}[\mathbf{F}^p)^{-1},\mathbf{I}] + (\mathbf{I}\otimes\nabla\tilde{\nu})[(\mathbf{F}^p)^{-1},\mathbf{I}]
\end{aligned}
\tag{38}
$$

- The mechanical power dissipated by the micro momentum associated with the plastic mechanism can be computed as

$$
\begin{aligned}
\nabla_{\mathcal{K}}\mathbf{L}^p\cdot\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p &= \sum_{\alpha=1}^{N}\{\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\nu^\alpha\}\cdot\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T} + \\
&+\sum_{\alpha=1}^{N}\{\mathbf{m}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\hat{\nu}^\alpha\}\cdot\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T} + (\mathbf{I}\otimes\nabla\tilde{\nu})\cdot\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T}.
\end{aligned}
\tag{39}
$$

- Let us introduce the plastic micro momentum with respect to the reference configuration, $\boldsymbol{\mu}_0^p$, by

$$\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p := (\mathbf{F}^p)^T \frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p[(\mathbf{F}^p)^{-T}, (\mathbf{F}^p)^{-T}]. \tag{40}$$

Consequently, the mechanical power dissipated by the micro plastic momentum given in (40) can be rewritten as

$$\begin{aligned} \nabla_{\mathcal{K}}\mathbf{L}^p \cdot \frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p &= \sum_{\alpha=1}^{N}\{\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha\} \cdot (\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T}\nabla\nu^\alpha) + \\ &+ \sum_{\alpha=1}^{N}(\mathbf{C}^p)^{-1}\{\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha\} \cdot \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p((\mathbf{F}^p)^{-T}\nabla\hat{\nu}^\alpha) + \mathbf{I} \cdot \frac{1}{\hat{\rho}}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T}\nabla\tilde{\nu}). \end{aligned} \tag{41}$$

when the fields are pulled back to the reference configuration.

- The micro forces $(g^d, \boldsymbol{\mu}^d)$ are related to the dislocation mechanism and are power conjugated with the rate of scalar dislocation density and its gradient, see (33). These micro forces satisfy the micro balance equation described by Cleja-Ţigoiu (2013)

$$\begin{aligned} &g^d = \operatorname{div}\boldsymbol{\mu}^d + \tilde{\rho}^d B^d, \iff \\ &J^p g^d = \operatorname{div}\boldsymbol{\mu}_0^d + \hat{\rho}_0 B^d, \quad \boldsymbol{\mu}_0^d = J^p(\mathbf{F}^p)^{-1}\boldsymbol{\mu}^d. \end{aligned} \tag{42}$$

Here B^d is mass density for the appropriate couple force. The last representation is written with respect to the reference configuration.

- We use the relationships between the micro momenta (42), the rate of the gradient of the dislocation density (30), as well as expressions of the rate of the plastic distortion (17) and (19) and we obtain

$$\begin{aligned} -\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^d \cdot \frac{1}{J^p}((\mathbf{F}^p)^{-1}\mathbf{L}^p)^T\, \nabla\rho^d &= -\sum_{\alpha=1}^{N}\nu^\alpha\,(\nabla\rho^d \cdot \hat{\mathbf{s}}^\alpha)(\hat{\mathbf{m}}^\alpha \cdot \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^d) - \\ -\sum_{\alpha=1}^{N}\hat{\nu}^\alpha\,(\nabla\rho^d\, \cdot (\mathbf{C}^p)^{-1}\hat{\mathbf{m}}^\alpha)(\hat{\mathbf{m}}^\alpha \cdot \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^d)\; &- \tilde{\nu}\,\nabla\rho^d \cdot \frac{\boldsymbol{\mu}_0^d}{\hat{\rho}_0}. \end{aligned} \tag{43}$$

- We use again the relationships between the micro momenta (42) and the continuity condition of the mass, namely $\tilde{\rho}\, J^p = \hat{\rho}_0$. We obtain the following representation

$$-\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^d \cdot \frac{1}{J^p}(\mathbf{F}^p)^{-T}\,\nabla\dot{\rho}^d = -\frac{1}{\hat{\rho}_0}\,\boldsymbol{\mu}^d. \tag{44}$$

Finally, the mechanical power dissipated by the micro stress momentum, $\boldsymbol{\mu}^d$ can be expressed, see for instance Cleja-Ţigoiu and Paşcan (2013b).

4 Elasto-Viscoplastic non-local Equations Compatible with the Free Energy Imbalance Principle

Theorem. 4 *The thermomechanical restriction imposed by the free energy imbalance principle is expressed as follows*

1. The elastic type constitutive equation written in terms of the Piola-Kirchhoff stress, $\boldsymbol{\pi}$, or the Cauchy stress tensor, $\mathbf{T}$, respectively, is characterized, in terms of the free energy density, by a potential

$$\frac{1}{\tilde{\rho}}\boldsymbol{\pi} = 2\,\partial_{\mathbf{C}^e}\psi_{\mathcal{K}} \quad \iff \quad \frac{1}{\hat{\rho}}\mathbf{T} = 2\mathbf{F}^e(\partial_{\mathbf{C}^e}\psi_{\mathcal{K}})\mathbf{F}^{eT}. \tag{45}$$

$\tilde{\rho}, \hat{\rho}$ are the mass densities with respect to the lattice state and current configuration.

Let us introduce the *generalized stress vector* in the plastically deformed configuration for the $\alpha-$slip system

$$\begin{aligned} &\mathbf{t}_{\hat{\mathbf{m}}^\alpha} := \boldsymbol{\Sigma}_0^p \hat{\mathbf{m}}^\alpha - (\hat{\mathbf{m}}^\alpha \cdot \boldsymbol{\mu}_0^d)\, \nabla \rho^d, \\ &t_{\mathbf{m}^0} = \boldsymbol{\Sigma}_0^p \cdot \mathbf{I} - \boldsymbol{\mu}_0^d \cdot \nabla \rho^d. \end{aligned} \tag{46}$$

The generalized stress vector involves the stress vector associated with Mandel's stress measure, $\boldsymbol{\Sigma}_0^p$, the gradient of the scalar dislocation density and the plastic micro momentum.

2. The dissipation inequality yields

$$\begin{aligned} &(\frac{1}{\hat{\rho}_0} g^d - \partial_{\rho^d}\psi) \cdot \dot{\rho}^d + (\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^d - \partial_{\nabla\rho^d}\ \psi) \cdot \nabla\dot{\rho}^d - \\ &-\frac{1}{\hat{\rho}_0}(g^d\rho^d + \mu_0^d \cdot \nabla\rho^d)(\sum_{\alpha=1}^{N} \hat{\nu^\alpha} + 3\tilde{\nu}^\alpha) + (\frac{1}{\hat{\rho}_0} t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}}\psi)\tilde{\nu} + \\ &+\sum_{\alpha=1}^{N}(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi)\nu^\alpha + \sum_{\alpha=1}^{N}(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot (\mathbf{C}^p)^{-1}\hat{\mathbf{m}}^\alpha - \partial_{\hat{\gamma}^\alpha}\psi)\hat{\nu}^\alpha + \\ &+\sum_{\alpha=1}^{N}\{(\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\gamma^\alpha}\psi\} \cdot \nabla\nu^\alpha + \\ &+\sum_{\alpha=1}^{N}\{(\mathbf{C}^p)^{-1}(\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\hat{\gamma}^\alpha}\psi\} \cdot \nabla\hat{\nu}^\alpha \\ &+(\mathbf{I} : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\tilde{\gamma}}\psi) \cdot \nabla\tilde{\nu} \geq 0. \end{aligned} \tag{47}$$

The product ":" is defined by the relationship (2).

In order **to simplify the constitutive relationships**, we adopt the method proposed by Grudmundson (2004),

The following **energetic constitutive equations** can be introduced

• The micro momentum associated with the dislocation mechanism, $\boldsymbol{\mu}_0^d$, is defined in terms of the free energy density as

$$\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^d - \partial_{\nabla\rho^d}\ \psi = 0. \tag{48}$$

Let $\mathcal{P}_t$ be the plastically deformed domain at a fixed moment of time. If we assume that the micro momentum on the boundary $\partial\mathcal{P}_t$ is oriented in the tangent direction, i.e. $\mathbf{m}_0^d \cdot \mathbf{N} = 0$, then the global dissipation realized by the set of fields $g^d\rho^d + \mu_0^\alpha \cdot \nabla\rho^d$,

$\int_{\partial\mathcal{P}_t}(g^d\rho^d + \mu_0^d \cdot \nabla\rho^d)dV = 0$, becomes zero due to the micro balance equation. This is the rationale to eliminate the third term in (47).

• The *micro momentum associated with the plastic mechanism*, $\boldsymbol{\mu}_0^p$, is described by its projections on the appropriate tensorial directions. This tensor field is given in order to satisfy the appropriate equalities

$$
\begin{aligned}
&(\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\gamma^\alpha}\psi = 0 \\
&(\mathbf{C}^p)^{-1}(\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\hat{\gamma}^\alpha}\psi = 0 \qquad (49)\\
&\mathbf{I} : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\tilde{\gamma}}\psi = 0
\end{aligned}
$$

The lattice vectors with respect to the reference configuration do not have the unit length and therefore we use the equivalent formulae associated with (49), but relative to the lattice configuration.

Proposition 2. The plastic micro momentum which satisfies the restriction written in the above formulae if and only if

$$
\begin{aligned}
\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p\ (\mathbf{F}^p)^{-T} \quad &= \sum_{\alpha=1}^{N}\big(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha\big) \otimes \partial_{\nabla\gamma^\alpha}\psi + \\
&+ \sum_{\alpha=1}^{N}\big(\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha\big) \otimes \partial_{\nabla\hat{\gamma}^\alpha}\psi + \mathbf{I} \otimes \partial_{\nabla\tilde{\gamma}}\psi
\end{aligned} \qquad (50)
$$

or equivalently

$$
\begin{aligned}
\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p \quad &= \sum_{\alpha=1}^{N}\big(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha\big) \otimes \mathbf{F}^p\ (\partial_{\nabla\gamma^\alpha}\psi) + \\
&+ \sum_{\alpha=1}^{N}\big(\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha\big) \otimes \mathbf{F}^p\ (\partial_{\nabla\hat{\gamma}^\alpha}\psi) + \mathbf{I} \otimes \mathbf{F}^p\ (\partial_{\nabla\tilde{\gamma}}\psi)
\end{aligned} \qquad (51)
$$

The dissipation inequality (47) is then reduced to

$$
\begin{aligned}
&(\frac{1}{\hat{\rho}_0}g^d - \partial_{\rho^d}\psi)\cdot\dot{\rho}^d + (\frac{1}{\hat{\rho}_0}t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}}\psi)\tilde{\nu} + \\
&+ \sum_{\alpha=1}^{N}(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi)\nu^\alpha + \sum_{\alpha=1}^{N}(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{m}}^\alpha - \partial_{\hat{\gamma}^\alpha}\psi)\hat{\nu}^\alpha \geq 0.
\end{aligned} \qquad (52)
$$

Consequently, the elastic type constitutive equation is given by (45), the energetic representation for the micro momenta are written in (48) and (51).

4.1 Rate Dependent Viscoplastic Model

We propose further a rate dependent viscoplastic models derived following the representation proposed in Gurtin and Anand (2005). The proposed model will be compatible with the dissipation inequality, given here by (52).

1. The *evolution equation for the dislocation density* will be taken in the form suggested by the dissipated power

$$
\dot{\rho}^d = \beta_1\big(\frac{g^d}{\hat{\rho}_0} - \partial_{\rho^d}\ \psi)\big), \qquad (53)
$$

   where β_1 is a scalar and positive valued function dependent on the process,

2. The *viscoplastic type constitutive relations* for the micro forces related with the plastic mechanism

$$
\begin{aligned}
\xi^\alpha \ \nu^\alpha \quad &= \big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi\big)\\
\hat\xi^\alpha \ \hat\nu^\alpha \quad &= \big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{m}}^\alpha - \partial_{\hat\gamma^\alpha}\psi\big)\\
\tilde\xi \ \tilde\nu \quad &= \big(\frac{1}{\hat\rho_0}t_{\mathbf{m}^0} - \partial_{\tilde\gamma}\psi\big).
\end{aligned}
\tag{54}
$$

3. The scalar constitutive function are defined in such a way to be compatible with the dissipation inequality (49)

$$
\beta_1(\dot\rho^d)^2 + \xi^\alpha\ (\nu^\alpha)^2 + \hat\xi^\alpha\ (\hat\nu^\alpha)^2 + \tilde\xi\ (\tilde\nu)^2 \geq 0.
\tag{55}
$$

The equivalent stress measure for α-slip system is defined by

$$
\tau^\alpha = \sqrt{\big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi\big)^2 + \big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{m}}^\alpha - \partial_{\hat\gamma^\alpha}\psi\big)^2 + \frac{1}{N^2}\big(\frac{1}{\hat\rho_0}t_{\mathbf{m}^0} - \partial_{\tilde\gamma}\psi\big)^2}
\tag{56}
$$

and the equivalent plastic rate

$$
\lambda^\alpha = \sqrt{(\nu^\alpha)^2 + (\hat\nu^\alpha)^2 + \frac{1}{N^2}\,(\tilde\nu)^2}
\tag{57}
$$

Let us introduce the assumption that functions $\xi^\alpha, \hat\xi^\alpha, \tilde\xi$ take equal values, which are proportional with $(\frac{\lambda^\alpha}{\lambda_0^\alpha})^m$, i.e.

$$
\begin{aligned}
\big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi\big) \quad &= \nu^\alpha S_Y\ (\frac{\lambda^\alpha}{\lambda_0^\alpha})^m\\
\big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{m}}^\alpha - \partial_{\hat\gamma^\alpha}\psi\big) \quad &= \hat\nu^\alpha S_Y(\frac{\lambda^\alpha}{\lambda_0^\alpha})^m\\
\big(\frac{1}{\hat\rho_0}t_{\mathbf{m}^0} - \partial_{\tilde\gamma}\psi\big) \quad &= \tilde\nu S_Y(\frac{\lambda^\alpha}{\lambda_0^\alpha})^m,
\end{aligned}
\tag{58}
$$

with S_Y and λ_0^α material parameters.

As a direct consequence of the constitutive relationships (58) the following equality holds

$$
(\tau^\alpha)^2 = S_Y^2\ (\lambda_0^\alpha)^2(\frac{\lambda^\alpha}{\lambda_0^\alpha})^{2(m+1)}, \text{or equivalently} \quad \frac{\lambda_0^\alpha}{\lambda^\alpha} = (\frac{\tau^\alpha}{S_Y\ \lambda_0^\alpha})^{\frac{1}{m+1}}
\tag{59}
$$

if the definitions (56) and (57) have been considered.

Viscoplastic constitutive equation If there exists a viscoplastic or an activation function $\mathcal{F} = \tau^\alpha - \zeta^\alpha$ the evolution equations for plastic components, compatible with the dissipation inequality, can be defined by

$$
\begin{aligned}
\nu^\alpha \quad &= \frac{\lambda_0^\alpha}{\lambda^\alpha}\big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi\big)\mathcal{H}(\tau^\alpha - \zeta^\alpha)\\
\hat\nu^\alpha \quad &= \frac{\lambda_0^\alpha}{\lambda^\alpha}\big(\frac{1}{\hat\rho_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot\hat{\mathbf{m}}^\alpha - \partial_{\hat\gamma^\alpha}\psi\big)\mathcal{H}(\tau^\alpha - \zeta^\alpha)\\
\tilde\nu^\alpha \quad &= \frac{\lambda_0^\alpha}{\lambda^\alpha}\big(\frac{1}{\hat\rho_0}t_{\mathbf{m}^0} - \partial_{\tilde\gamma}\psi\big)\mathcal{H}(\tau^\alpha - \zeta^\alpha),
\end{aligned}
\tag{60}
$$

with $\frac{\lambda_0^\alpha}{\lambda^\alpha}$ expressed in terms of the stress by $(59)_2$, and the evolution equation for the dislocation density has been written in (53).

Conclusion. We summarize the description of the model, which is strongly dependent on the free energy density expression, written in (32), say under the form

$$\psi = \frac{1}{2}\mathbf{C}^e \cdot \mathcal{E}(\mathbf{C}^e) + \psi^d(\gamma^\alpha, \hat{\gamma}^\alpha, \tilde{\gamma}, \nabla\gamma^\alpha, \nabla\hat{\gamma}^\alpha, \nabla\tilde{\gamma}, \rho^d, \nabla\rho^d). \tag{61}$$

- elastic type constitutive equation is derived from (45)

$$\mathbf{T} = 2\hat{\rho}\mathbf{F}^e\mathcal{E}(C^e - \mathbf{I})\mathbf{F}^{eT} \tag{62}$$

- viscoplastic constitutive relations written in (60) together with (59) and (56), where $\mathbf{t}_{\hat{\mathbf{m}}^\alpha}$ and $\mathbf{t}_{\mathbf{m}_0}$ are defined in (46) in terms of $\mathbf{\Sigma}_0^p\hat{\mathbf{m}}^\alpha$ and $\boldsymbol{\mu}_0^d$;
- the Mandel type stress measure related to plastic behaviour is given by the relationships (36) together with (35)

$$\frac{1}{\hat{\rho}_0}\mathbf{\Sigma}_0^p = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^T\big(\ \mathrm{div}\ (J^p\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T})\big)(\mathbf{F}^p)^{-T}, \tag{63}$$

  while $J^p\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T}$ is described by an energetic relationship given by (50).

- $\boldsymbol{\mu}_0^d$ is given by (48), $\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^d - \partial_{\nabla\rho^d}\ \psi = 0.$
- Finally the evolution equation for the hardening parameters ζ^α (as for instance in Teodosiu and Sidoroff (1976), which enter the expression of viscoplastic equations (60) through the activation function.
- The non local evolution for the scalar dislocation density is defined by (53), together (42) and (48)

$$\dot{\rho}^d = \beta_1\big(\frac{1}{\hat{\rho}_0}\mathrm{div}\,\hat{\rho}_0\partial_{\nabla\rho^d}\ \psi - \partial_{\rho^d}\ \psi\big) \tag{64}$$

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