MULTI-SLIP AND NON-LOCAL EVOLUTION EQUATIONS IN FINITE ELASTO-PLASTIC MATERIALS WITH DISLOCATIONS

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Abstract. The paper deals with elasto-plastic models which describe the behaviour at large strain of materials with crystalline structure, which contain continuously distributed dislocations. The non-local evolution equations for dislocation densities are derived to be compatible with the the principle of free energy imbalance, when a non-Schmid flow rule describes the evolution of the plastic distortion within the crystalographic systems. We analyze the constitutive restrictions that follow from the principle of the free energy imbalance for the case when the free energy density is dependent on the scalar dislocation densities and their gradients, and for a more general case when the influence of the tensorial measure of dislocations is considered too.

Key words: dislocations, non-Schmid flow rule, crystalline materials, non-local evolution equations, finite elasto-plasticity.

1. INTRODUCTION

The paper deals with elasto-plastic materials with crystalline structure containing continuously distributed defects, 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 [33], Mandel [31]. In order to define the plastic part of the deformation gradient, a local stress free (relaxed) configuration is associated with a given material point. These local stress free configurations become incompatible, and in order to restore a continuous body it is necessary to deform elastically these relaxed configurations. The multiplicative decomposition of the deformation gradient into its elastic and plastic components have been introduced, see Teodosiu [33], Mandel [31], and models with local relaxed configurations and internal variables were developed by Cleja-Ţigoiu [7], Cleja-Ţigoiu and Soós [6].

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The geometry of the material structure with defects is characterized by the so-called plastic distortion and plastic connection, following Kondo and Yuki [25], Bilby [2], Kröner [26], [27], within a second order plasticity, namely when the gradient of the deformation gradient has to be considered. The pair of the so-called plastic distortion, $\mathbf{F}^p$, which are incompatible and plastic connection, $\overset{(p)}{\mathbf{\Gamma}}$, are introduced, together with the multiplicative decomposition of the deformation gradient and the transformation rule of the connections, see Cleja-Ţigoiu [9], [11] and [16]. We postulated that the so-called plastic connection has non-zero Cartan torsion, see Bilby [2], Kondo and Yuki [25], de Wit [19]. The Cartan torsion is viewed as a tensorial measure of dislocations, which is sometimes called *the defect density tensor*, or *geometrically necessary dislocations*.

The constitutive models provided here are compatible with the free energy imbalance principle, formulated by Cleja-Ţigoiu [9], [11], following Gurtin [22], Gurtin et al. [24]. The constitutive description is first formulated with respect to the crystal lattice configuration and is strongly dependent on the expression assumed for the free energy density function. The key point is the postulate of the imbalance of the free energy, developed within the second order plasticity. Within the constitutive framework proposed by Cleja-Ţigoiu [9], [11] and [12], the micro forces, namely micro stress and micro stress momenta related to the plastic mechanism and the defects, resoectively, produce an internal power. A model with Schmid flow rule and with non-local evolution equations for the scalar dislocation densities and non-local back stress, was derived by Cleja-Ţigoiu and Paşcan [13], as a naturale generalizetion of the model developped by Teodosiu et al. [35].

Here we start from the supposition that the non-Schmid flow rule describes the evolution of the plastic distortion, as Kuroda [30], Dao and Asaro [18] and Cleja-Ţigoiu and Paşcan [14] considered. In the model proposed by Cleja-Ţigoiu and Paşcan [14], the rate of plastic distortion involves not only the shear rates but also 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. In the model proposed by Cleja-Ţigoiu [17] the influence of the dislocation density tensor $\mathbf{G}$, which is different from the (GND) dislocation tensor defined by Cermelli and Gurtin [4], is considered. The formula which expresses the time derivative of $\mathbf{G}$ is provided 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.

Our goal is to provide the non-local evolution equations for the components of plastic distortion and the scalar dislocation densities for crystalline materials, which are compatible with the imbalance of the free energy density. We assume that that the plastic deformation of elasto-plastic materials with crystalline structure is described by the multi-slip on the appropriate crystalographic systems, using a modified Schmid flow rule. We analyze the constitutive restrictions resulting from the assumption that the non-Schmid law occurs and compare the models, developped by Cleja-Ţigoiu and Paşcan [14], and Cleja-Ţigoiu [17].

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 second and third order tensors, respectively, defined 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 $\mathbf{u}\in\mathscr{V}$.
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 $\mathbf{a}\in\mathscr{V}$, is a third order tensor, with the property
$(\mathbf{A}\otimes\mathbf{a})\mathbf{v} = \mathbf{A}(\mathbf{a}\cdot\mathbf{v}), \quad (\mathbf{A}\cdot(\mathbf{a}\otimes\mathbf{v}) = \mathbf{a}\cdot(\mathbf{A}\mathbf{v}), \forall\mathbf{v}\in\mathscr{V}.$

$\mathbf{I}$ 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:

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

$Lin(\mathscr{V}, Lin) = \{\mathbf{N}:\mathscr{V}\longrightarrow Lin, \quad \text{linear}\}-$ defines the space of all third order tensors and it is given by $\mathbf{N} = N_{ijk}\mathbf{i}^i\otimes\mathbf{i}^j\otimes\mathbf{i}^k$.
The scalar product of two second order tensor $\mathbf{A},\mathbf{B}$ is $\mathbf{A}\cdot\mathbf{B} := \mathrm{tr}(\mathbf{A}\mathbf{B}^T) = A_{ij}B_{ij}$, 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 $\mathbf{A} : \mathbf{M}$

$$(\mathbf{A} : \mathbf{M})\cdot\mathbf{u} = \mathbf{A}\cdot(\mathbf{M}\mathbf{u}), \;\forall\,\mathbf{u}\in\mathscr{V} \tag{2}$$

The gradient in a local coordinate for a vector, $\mathbf{Y}$, second order tensor, $\mathbf{C}$, and are denoted by

$$\nabla\mathbf{Y} = \frac{\partial Y^a}{\partial x^b}\mathbf{e}_a\otimes\mathbf{e}^b, \quad \nabla\mathbf{C} = \frac{\partial C_{lm}}{\partial x^k}\mathbf{e}^l\otimes\mathbf{e}^m\otimes\mathbf{e}^k. \tag{3}$$

The *divergence* operator acts on second and third order tensors, $\mathbf{T}$ and $\mathbf{N}$, respectively, as

$$div\mathbf{T} = \frac{\partial T_{im}}{\partial x^m}\mathbf{e}^i, \quad div\mathbf{N} = \frac{\partial N_{ijm}}{\partial x^m}\mathbf{e}^i\otimes\mathbf{e}^j. \tag{4}$$

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

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

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

$$\begin{aligned} &\mathscr{A} \cdot \mathscr{B}\mathbf{F}_1 = \mathscr{A}\mathbf{F}_1^T \cdot \mathscr{B} \\ &(\mathscr{A}[\mathbf{F}_1, \mathbf{F}_2])[\mathbf{F}_3, \mathbf{F}_4] = (\mathscr{A}[\mathbf{F}_1\mathbf{F}_3,\, \mathbf{F}_2\mathbf{F}_4] \end{aligned} \tag{6}$$

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

Let $\mathbf{F}(\mathbf{X},t) = \nabla\chi(\mathbf{X},t)$ be the deformation gradient at time t, $\mathbf{X} \in \mathscr{B}$, were $\chi(\cdot,\cdot)$ denotes the motion of the body $\mathscr{B}$.

AXIOM 1. *We assume that the deformation gradient is multiplicatively decomposed into its elastic and plastic components, called distortions, namely*

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p. \tag{8}$$

The plastic distortion $\mathbf{F}^p$ characterizes the local deformation from the reference configuration to the so-called isoclinic configuration. In order to define correctly, on a physical basis, the elastic and plastic distortions we use the so-called isoclinic configuration introduced by Teodosiu [33], Mandel [31]. The elastic distortion $\mathbf{F}^e$ describes the local mapping from the *isoclinic configuration* to the deformed configuration. The indetermination in choosing the local relaxed configuration, which is attached to the crystalline lattice, has been eliminated by assuming that, in these isoclinic configurations, the corresponding crystalline directions are parallel to each other. The isoclinic configurations are uniquelly associated to the motion, apart from orthogonal trasnformations which are elements of the material symmetry group, at the given material points of the body. We adopted the constitutive framework of elasto-plastic materials with relaxed configurations and internal state variables, which has been proposed by Cleja-Ţigoiu [7], and Cleja-Ţigoiu and Soós [6].

In this paper three configurations will be considered:

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

• $\chi(\cdot,t)$ the deformed configuration at time t, where $\chi :\to \mathscr{E}$ defines the motion of the body $\mathscr{B}$,

• the isoclinic (anholonomic) configuration related to the lattice structure, denoted $\mathscr{K}$, associated to the plastically deformed configuration.

The geometry of the plastically deformed configuration is characterized by the plastic distortion $\mathbf{F}^p$, which is incompatible tensorial field, i.e. *curl*$\mathbf{F}^p$ is non-vanishing, and by a plastic connection which has metric property and is reduced to a Bilby type connection.

In [11] it is proved that

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

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

$\overset{(\mathrm{p})}{\mathscr{A}}$ is Bilby's type connection and $\mathbf{\Lambda}$ denotes the *disclination (second order) tensor*.

We restrict here to the case $\mathbf{\Lambda} = 0$, which has been considered in [8] and geometrically analyzed by Cleja-Ţigoiu et al. [10].

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

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

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

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

THEOREM. *The second order torsion tensor,* $\mathscr{N}^p$, *denoted here by* $\boldsymbol{\alpha}$, *associated with the Cartan torsion, is expressed by*

$$\boldsymbol{\alpha} = (\mathbf{F}^p)^{-1} \mathrm{curl} \mathbf{F}^p. \tag{11}$$

This second order field $\boldsymbol{\alpha}$ has been introduced by Noll [32] as a tensorial measure of dislocations.

We remark that there exists an *anholonomic configuration*, $\mathscr{K}$, which is associated with the second order plastic deformation, namely $(\mathbf{F}^p, \overset{(\mathrm{p})}{\mathbf{\Gamma}})$. The gradient in the configuration $\mathscr{K}$ of the field $\mathbf{F}$, $\nabla_{\mathscr{K}} \mathbf{F}$, is calculated by

$$\nabla_{\mathscr{K}} \mathbf{F} := (\nabla \mathbf{F})(\mathbf{F}^p)^{-1}, \tag{12}$$

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

As a direct consequence of the multiplicative decomposition of the deformation gradient into its components, (8), 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

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e\mathbf{L}^p\,(\mathbf{F}^e)^{-1}, \quad \mathbf{L}^e = \dot{\mathbf{F}}^e\,(\mathbf{F}^e)^{-1}, \quad \mathbf{L}^p = \dot{\mathbf{F}}^p\,(\mathbf{F}^p)^{-1}. \tag{13}$$

Note that in contrast to the rate of plastic distortion, which is related to the local relaxed configuration (or the plastically deformed configuration), the velocity gradient and rate of the elastic distortion are related to the current deformed configuration.

Within the constitutive framework of finite elasto-plasticity with second order deformation, the paper by Cleja-Ţigoiu [12] proposes the models with

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

Remark. Only the skew-symmetric part of $\overset{(\mathrm{p})}{\mathscr{A}}$ enters the definition of the tensorial measure of dislocation density $\boldsymbol{\alpha}$, as can be seen from (9)-(11), written for $\boldsymbol{\Lambda} = 0$.

In the present paper models with scalar and tensorial dislocation densities are presented.

Let us introduce the scalar dislocation density with respect to the lattice configuration $\rho^d_{\mathscr{K}}$ and its gradient, which are related with whose related to the reference configuration, ρ and $\nabla\rho$, respectively, by

$$\begin{aligned} &\rho^d_{\mathscr{K}} = \frac{1}{J^p}\rho^d \\ &\nabla_{\mathscr{K}}\rho^d_{\mathscr{K}} := \frac{1}{J^p}(\mathbf{F}^p)^{-T}\nabla\rho^d, \quad J^p = \mid \det\mathbf{F}^p \mid \end{aligned} \tag{14}$$

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

$$\begin{aligned} &\frac{d}{dt}\rho^d_{\mathscr{K}} = \frac{1}{J^p}(\dot{\rho}^d - \rho^d\,\mathrm{tr}\mathbf{L}^p), \\ &J^p\,\frac{d}{dt}(\nabla_{\mathscr{K}}(\rho^d_{\mathscr{K}})) = -\mathrm{tr}\,\mathbf{L}^p(\mathbf{F}^p)^{-T}\nabla\rho^d - ((\mathbf{F}^p)^{-1}\mathbf{L}^p)^T\,\nabla\rho^d + (\mathbf{F}^p)^{-T}\nabla\dot{\rho}^d. \end{aligned} \tag{15}$$

2.1. MODEL WITH SCHMID PLASTIC EVOLUTION LAW

In **crystal plasticity**, the rate of plastic distortion is defined by multislips in the appropriate crystallographic system (i.e. isoclinic configuration)

$$\dot{\mathbf{F}}^p\left(\mathbf{F}^p\right)^{-1}=\sum_{\alpha=1}^{N}\dot{\gamma}^{\alpha}(\bar{\mathbf{s}}^{\alpha}\otimes\bar{\mathbf{m}}^{\alpha}), \tag{16}$$

where $\dot{\gamma}^{\alpha}$ is the plastic shear rate in the slip system α. The slip system initially given in the lattice configuration, where $\bar{\mathbf{m}}^{\alpha}$ is the normal to the slip plane and $\bar{\mathbf{s}}^{\alpha}$ is the slip direction, is further deformed due to the presence of the elastic distortion $\mathbf{F}^e$. In the actual configuration the slip system, $(\mathbf{m}^{\alpha},\mathbf{s}^{\alpha})$, is defined by the following formulae

$$\mathbf{s}^{\alpha}=\mathbf{F}^e\bar{\mathbf{s}}^{\alpha},\quad \mathbf{m}^{\alpha}=\left(\mathbf{F}^e\right)^{-T}\bar{\mathbf{m}}^{\alpha}. \tag{17}$$

The orthogonality condition, $\mathbf{s}^{\alpha}\cdot\mathbf{m}^{\alpha}=0$, obviously holds.

Hence the **rate of elastic distortion** can be expressed, from (13) together with (16), in the actual configuration, in terms of the velocity gradient $\mathbf{L}$ as

$$\dot{\mathbf{F}}^e\left(\mathbf{F}^e\right)^{-1}=\mathbf{L}-\sum_{\alpha=1}^{N}\dot{\gamma}^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right),\quad \mathbf{L}=\dot{\mathbf{F}}\left(\mathbf{F}\right)^{-1}, \tag{18}$$

and we note that

$$\mathbf{F}^e\dot{\mathbf{F}}^p(\mathbf{F}^p)^{-1}(\mathbf{F}^e)^{-1}=\sum_{\alpha=1}^{N}\dot{\gamma}^{\alpha}\left(\mathbf{s}^{\alpha}\otimes\mathbf{m}^{\alpha}\right). \tag{19}$$

The following internal variables are used herein:

the dislocation densities ρ^{α} and hardening variables (or slip resistances) ζ^{α} in the $\alpha-$slip system, which are described by appropriate evolution equations.

The model will be strongly related to the presence, production and motion of dislocations inside the body.

The **activation condition** is formulated in terms of the Schmid law

$$|\tau^{\alpha}-\tau_b^{\alpha}|\geq\zeta^{\alpha}\quad\Longleftrightarrow\quad\mathscr{F}^{\alpha}\geq 0\quad\text{where}\quad\mathscr{F}^{\alpha}:=|\tau^{\alpha}-\tau_b^{\alpha}|-\zeta^{\alpha}, \tag{20}$$

where τ^{α} is the *reduced shear stress in the* $\alpha-$ *slip system* or the *resolved shear stress*

$$\begin{aligned}&\tau^{\alpha}=\boldsymbol{\tau}\mathbf{m}^{\alpha}\cdot\mathbf{s}^{\alpha},\\&\boldsymbol{\tau}=J\mathbf{T},\quad\text{where}\quad J=\det\mathbf{F}\equiv\frac{\hat{\rho}_0}{\hat{\rho}}.\end{aligned} \tag{21}$$

A *viscoplastic flow* rule associated with the deformation process is given in the form in [34]

$$v^\alpha = \dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left| \frac{\tau^\alpha - \tau_b^\alpha}{\zeta^\alpha} \right|^n \operatorname{sign}(\tau^\alpha)\mathscr{H}\mathscr{F}^\alpha), \quad \forall \alpha = 1,...,N. \tag{22}$$

The *hardening law* is described either by a given function dependent on the dislocation densities like $\zeta^\alpha = \mu b \left(\sum_\beta a^{\alpha\beta} \rho^\beta \right)^{1/2}$ [34], where μ is the elastic shear modulus, b is the magnitude of the Burgers vector, $\left(a^{\alpha\beta}\right)$ - the matrix taking into account various types of dislocation interactions, or an evolution law proposed like in crystal plasticity in terms of plastic shear rates [35]

$$\dot{\zeta}^\alpha = \sum_{\beta=1}^{N} h^{\alpha\beta} \left| \dot{\gamma}^\beta \right|. \tag{23}$$

Here $h^{\alpha\beta} = h^{\alpha\beta}(\rho^q)$ are the components of the hardening matrix and they depend on the dislocation density. Moreover, this matrix has been represented by Teodosiu et al. [35] as

$$h^{\alpha\beta} = \frac{\mu}{2} a^{\alpha\beta} \left(\sum_q a^{\alpha q} \rho^q \right)^{-1/2} \left\{ \frac{1}{K} \left(\sum_{q \neq \alpha} \rho^q \right)^{1/2} - 2 y_c \rho^\alpha \right\}, \tag{24}$$

where K is a material parameter and y_c denotes a characteristic length associated with the annihilation process of dislocation dipoles.

Remark. Asaro and Needleman [1] proposed the expression for the hardening moduli

$$h^{\alpha\beta} = q^{\alpha\beta} h^\beta, \quad h^\beta = h_s + (h_0 - h_s)\operatorname{sech}^2 \left(\frac{h_0 - h}{\tau_s - \tau_0} \right) \gamma_a \tag{25}$$

where τ_s represents the saturation value of the shear stress, h_0, h_s are the initial and asymptotic hardening rates and γ_a is the accumulated shear strain, and in the influence matrix $\{q^{\alpha\beta}\}_{\alpha\beta}$ $q^{\alpha\beta}$ equals unity for coplanar slip systems and the scalar value q for non-coplanar systems. In Evens et al. [20] $h^\beta = h_0(1 - \frac{s_\beta}{s_\infty})$, with the slip hardening parameters. In the numerical algorithm proposed in this paper the slip rates, $\dot{\gamma}^\alpha$ are computed using the equation (22) together with the implicit in time integration of the equation (23). At a given stress state the slip rates are solved by Newton-Raphson method. The hardening parameters, called slip system resistances, are also solved using Newton-Raphson procedure. In the numerical algorithm the derivative of the slip rates with respect to stress are also required.

Various scalar and tensorial dislocation densities were introduced in order to describe the behaviour of elasto-plastic materials with dislocations. We present here possible evolution equations for the scalar dislocation densities, which are related with our proposed models.

The evolution in time of the dislocation densities is described either by *a local* evolution equation, or by *non-local laws* which account for the size effect.

I. We consider the *local evolution equation*, say of the such type as given in [35]

$$\dot{\rho}^{\alpha} = \frac{1}{b}\left(\frac{1}{L^{\alpha}} - 2y_c\rho^{\alpha}\right)|v^{\alpha}| \quad \text{cu} \quad L^{\alpha} = K\left(\sum_{q\neq\alpha}\rho^{q}\right)^{-1/2} \tag{26}$$

II. A *non local evolution equation*, namely a diffusive evolution equation, [3] which is non-linear and of the parabolic type

$$\dot{\rho}^{\alpha} = D\left(k\Delta\rho^{\alpha} - \frac{\partial\psi_T}{\partial\rho^{\alpha}}\right)|v^{\alpha}|, \quad \alpha = 1,\ldots,N, \tag{27}$$

where D, k are material constants. Here Ψ_T represents the defect energy.

Remark. In the paper [15], an appropriate expression for the potential ψ_T was identified by considering the equality between the functions in the right hand side of equations (16) and (17) with $k = 0$, namely

$$\psi_T = y_c(\rho^{\alpha})^2 - \frac{1}{K}\left(\sum_{\beta\neq\alpha}\rho^{\beta}\right)^{1/2}\rho^{\alpha}. \tag{28}$$

III. The non-local evolution laws used in [29], [28] assert that the variation in time of the dislocation densities, namely $\rho^{(\alpha)}_{G(e)}, \rho^{(\alpha)}_{G(s)}$, is proportional to the projection of the gradient of the plastic shear rate on the normal and slip direction, respectively. The evolution equations are governed by the following differential equations

$$\dot{\rho}^{(\alpha)}_{G(e)} = -\frac{1}{b}\mathrm{grad}\nu^{(\alpha)}\cdot\bar{\mathbf{s}}^{(\alpha)}, \quad \dot{\rho}^{(\alpha)}_{G(s)} = -\frac{1}{b}\mathrm{grad}\nu^{(\alpha)}\cdot\bar{\mathbf{p}}^{(\alpha)}, \tag{29}$$

where $\bar{\mathbf{s}}^{(\alpha)}$ and $\bar{\mathbf{p}}^{(\alpha)}$ are considered in the deformed configuration. The edge and screw GND densities on the slip system, namely $\rho^{(\alpha)}_{G(e)}, \rho^{(\alpha)}_{G(s)}$, characterize the geometrically necessary dislocations (GND) via the expression developed as for instance in Cermelli and Gurtin [4]

$$\begin{gathered}\overset{\diamond}{\mathbf{G}} = b\sum_{\alpha}(-\dot{\rho}^{(\alpha)}_{G(e)}\mathbf{p}^{(\alpha)}\otimes\mathbf{s}^{(\alpha)} + \dot{\rho}^{(\alpha)}_{G(s)}\mathbf{s}^{(\alpha)}\otimes\mathbf{s}^{(\alpha)}),\\ \text{where} \quad \overset{\diamond}{\mathbf{G}} = \dot{\mathbf{G}} - \mathbf{L}^{p}\mathbf{G} - \mathbf{G}(\mathbf{L}^{p})^{T}.\end{gathered} \tag{30}$$

The rate of macroscopic distribution of screw and edge dislocations were introduced in [4] as the coefficients of the appropriate tensorial products.

In the papers by [29], [28] the gradient of the dislocation densities $\rho^{(\alpha)}_{G(e)}, \rho^{(\alpha)}_{G(s)}$ are involved into the definition adopted for the back stress relation that neglect interactions between the slip systems

$$\tau_b^{(\alpha)} = b\tau_0 L^2 \big(\mathrm{grad}\bar{\rho}^{(\alpha)}_{G(e)} \cdot \bar{\mathbf{s}}^{(\alpha)} + \mathrm{grad}\bar{\rho}^{(\alpha)}_{G(s)} \cdot \bar{\mathbf{p}}^{(\alpha)}\big), \tag{31}$$

L is a scale length parameter, $\bar{\rho}^{(\alpha)}_{G(e)} = J^{-1}\rho^{(\alpha)}_{G(e)}$ and $\bar{\rho}^{(\alpha)}_{G(s)} = J^{-1}\rho^{(\alpha)}_{G(s)}$.

Let us remark here that the models presented in (Kuroda and Tvergaard [29] and Kuroda [28] no higher-order microscopic stress has been involved. The last mentioned paper is an extension to finite deformation of the small deformation models previously proposed.

A non-local evolution equation for the dislocation density dependent on its gradient has been derived in [13]. In the constitutive framework considered by Cleja-Ţigoiu and Paşcan [15], the back stress on the slip system α denoted by τ_b^α was defined by

$$\tau_b^\alpha = \kappa_2(\bar{\mathbf{s}}^\alpha \cdot \nabla\rho^\alpha)(\bar{\mathbf{m}}^\alpha \cdot \nabla\rho^\alpha), \tag{32}$$

with κ_2 involving a length scale parameter, in terms of the gredients of the dislocation densities, following [13].

2.2. NON-SCHMID PLASTIC EVOLUTION EQUATIONS

The evolution equation for the plastic distortion is given by a modified form of those traditionally considered in crystal plasticity, (16). A priori we do not make any assumption on the relationships between these scalar plastic velocities as was done by Kuroda [30].

AXIOM 2. *The evolution equation for the plastic distortion is given in a form that involves not only the shear in the slip system, but also the normal velocity to the slip system*

$$\dot{\mathbf{F}}^p\,(\mathbf{F}^p)^{-1} = \sum_{\alpha=1}^{N} \nu^\alpha\,(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha) + \sum_{\alpha=1}^{N} \hat{\nu}^\alpha\,(\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha) + \tilde{\nu}\,\mathbf{I}, \tag{33}$$

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 plastic volume expansion and $\mathbf{I}$ *is the second order identity tensor.*

In what follows we assume **the plastic compressibility**, i.e. $J^p := \mid \det\mathbf{F}^p \mid \neq 1$, since as a direct consequence of formula (33), $\mathrm{tr}(\mathbf{L}^p)$ could be estimated as

$$\mathrm{tr}(\mathbf{L}^p) = \hat{\nu} + 3\,\tilde{\nu}, \quad \text{where} \quad \hat{\nu} = \sum_{\alpha=1}^{N} \nu^\alpha \tag{34}$$

The directions of the $\alpha-$slip system, $(\mathbf{s}^\alpha, \mathbf{m}^\alpha)$, are considered to be fixed with respect to the reference configuration as a consequence of the supposition that the relaxed configurations are isoclinic, see e.g. Mandel [31] and Teodosiu [33], which means that the crystal lattice has the same orientation in the relaxed and reference configurations. The slip system is deformed during the plastic deformation as follows:

$$\begin{array}{lll} \hat{\mathbf{s}}^\alpha = (\mathbf{F}^p)^{-1}\mathbf{s}^\alpha, & \hat{\mathbf{m}}^\alpha = (\mathbf{F}^p)^T\,\mathbf{m}^\alpha, & \text{in the reference configuration,} \\ \bar{\mathbf{s}}^\alpha = \mathbf{F}^e\,\mathbf{s}^\alpha, & \bar{\mathbf{m}}^\alpha = (\mathbf{F}^e)^{-T}\,\mathbf{m}^\alpha, & \text{in the actual configuration,} \end{array} \tag{35}$$

where $\hat{\mathbf{s}}^\alpha$ and $\bar{\mathbf{s}}^\alpha$ represent the glide vectors and $\hat{\mathbf{m}}^\alpha, \bar{\mathbf{m}}^\alpha$ are vectors parallel to the transformed normal vectors via Nanson's formula, say e.g. $(\det \mathbf{F}^p)\,(\mathbf{F}^p)^{-T}\,\hat{\mathbf{m}}^\alpha$, in the appropriate configurations. Clearly, $\hat{\mathbf{s}}^\alpha \cdot \hat{\mathbf{m}}^\alpha = 0$ and $\bar{\mathbf{s}}^\alpha \cdot \bar{\mathbf{m}}^\alpha = 0$.

• Kuroda [30] proposed the following representation (according to the present notation) for the rate of the plastic distorsion, which contains terms in the normal direction and is pressure dependent; this fact has been described directly in the deformed configuration via the following relations

$$(\mathbf{F}^e)\dot{\mathbf{F}}^p\,(\mathbf{F}^p)^{-1}\,(\mathbf{F}^e)^{-1} = \mathbf{D}^p + \mathbf{W}^p; \quad \mathbf{W}^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha\,\{(\bar{\mathbf{s}}^\alpha \otimes \overline{\mathbf{m}}^\alpha)\}^a$$

$$\begin{aligned} \mathbf{D}^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha\,\{(\bar{\mathbf{s}}^\alpha \otimes \overline{\mathbf{m}}^\alpha)\}^S + \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha\,\mathrm{sgn}(\dot{\gamma}^\alpha)\,(\overline{\mathbf{m}}^\alpha \otimes \overline{\mathbf{m}}^\alpha) + \\ + d\,\dot{\gamma}^\alpha\,\mathrm{sgn}(\dot{\gamma}^\alpha) \sum_{\alpha=1}^{N} \mid \nu^\alpha \mid \mathbf{I}, \end{aligned} \tag{36}$$

where N is the number of slip-systems, $\dot{\gamma}^\alpha$ is the slip velocity on the $\alpha-$slip system, and d is a material parameter that characterizes the plastic compressibility effect. Here $(\overline{\mathbf{m}}^\alpha, \bar{\mathbf{s}}^\alpha)$ defines the slip system *in the deformed configuration*. The flow rule for each slip system is finally related to $\mid \tau^\alpha \mid$.

Let us introduce the rate of plastic distorsion with respect to the reference configuration, namely

$$\hat{\mathbf{l}}^p := (\mathbf{F}^p)^{-1}\dot{\mathbf{F}}^p = (\mathbf{F}^p)^{-1}\,\mathbf{L}^p\,\mathbf{F}^p \tag{37}$$

and its representation follows at once as a consequence of (33) and (37)

$$\hat{\mathbf{l}}^p = \sum_{\alpha=1}^{N} \nu^\alpha\,(\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) + \sum_{\alpha=1}^{N} \hat{\nu}^\alpha\,\left(\mathbf{C}^p\right)^{-1}(\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha\right) + \tilde{\nu}\,\mathbf{I}, \quad \mathbf{C}^p = (\mathbf{F}^p)^T\mathbf{F}^p. \tag{38}$$

The Bilby type plastic connection $\overset{(\mathrm{p})}{\mathscr{A}}$ with respect to the reference configuration is defined in terms of the gradient of the plastic distortion in (9) by

$$\overset{(\mathrm{p})}{\mathscr{A}} := (\mathbf{F}^p)^{-1}\nabla\mathbf{F}^p. \tag{39}$$

When the time derivative of (39) is taken, in the hypothesis concerning the expression of the rate of plastic distorsion (33), one obtains

$$\begin{aligned} \frac{d}{dt}(\overset{(\mathrm{p})}{\mathscr{A}}) &= \sum_{\alpha=1}^{N} (\mathbf{F}^p)^{-1}\{\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \otimes \nabla\nu^\alpha\}[\mathbf{I},\mathbf{F}^p] + \\ &+ \sum_{\alpha=1}^{N} (\mathbf{F}^p)^{-1}\{\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha \otimes \nabla\hat{\nu}^\alpha\}[\mathbf{I},\mathbf{F}^p] + (\mathbf{I}\otimes\nabla\tilde{\nu}). \end{aligned} \tag{40}$$

Remark. The rate of plastic distortion has been postulated in (33) to be given by the slip mechanism with respect to the isoclinic configuration and not the expression of the plastic distortion itself. Consequently, the rate of the Bilby type plastic connection can be provided only, following Cleja-Ţigoiu [17].

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

$$\begin{aligned} &\mathbf{G} \equiv \boldsymbol{\alpha} = (\mathbf{F}^p)^{-1}\mathrm{curl}\mathbf{F}^p, \text{or its equivalent expression} \\ &\mathbf{G}(\mathbf{u}\times\mathbf{v}) = (\overset{(\mathrm{p})}{\mathscr{A}}\,\mathbf{u})\mathbf{v} - (\overset{(\mathrm{p})}{\mathscr{A}}\,\mathbf{v})\mathbf{u} \end{aligned} \tag{41}$$

that holds for any vector fields $\mathbf{u},\mathbf{v}$. Our formulae written in (41) have been already derived through (9)- (11). In order to compute the time derivative of (GND)- dislocation density we start from the relationship

$$(\frac{d}{dt}\mathbf{G})(\mathbf{u}\times\mathbf{v}) = ((\frac{d}{dt}\overset{(\mathrm{p})}{\mathscr{A}})\mathbf{u})\mathbf{v} - (\frac{d}{dt}\overset{(\mathrm{p})}{\mathscr{A}}\,\mathbf{v})\mathbf{u}, \tag{42}$$

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 $\mathbf{G}$ can be expressed by

THEOREM(Cleja-Ţigoiu [17]).

$$\frac{d}{dt}\mathbf{G} = \sum_{\alpha=1}^{N} \frac{1}{\mid \hat{\mathbf{s}}^\alpha \mid^2} (\nabla v^\alpha \cdot \hat{\mathbf{s}}^\alpha)\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{p}}^\alpha - \sum_{\alpha=1}^{N} \frac{1}{\mid \hat{\mathbf{s}}^\alpha \mid^2} (\nabla v^\alpha \cdot \hat{\mathbf{p}}^\alpha)\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{s}}^\alpha +$$

$$+(\mathbf{C})^{-1} \sum_{\alpha=1}^{N} \frac{1}{\mid \hat{\mathbf{s}}^\alpha \mid^2} \big((\nabla \hat{v}^\alpha \cdot \hat{\mathbf{s}}^\alpha)\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{p}}^\alpha - (\nabla \hat{v}^\alpha \cdot \hat{\mathbf{p}}^\alpha)\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{s}}^\alpha\big) + \in \nabla \tilde{v}, \tag{43}$$

$$\text{where} \quad \mid \hat{\mathbf{s}}^\alpha \mid^2 = \hat{\mathbf{s}}^\alpha \cdot \mathbf{c}^p \hat{\mathbf{s}}^\alpha, \quad \mathbf{c}^p = (\mathbf{F}^p)^{-T}(\mathbf{F}^p)^{-1}.$$

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

$$((\mathbf{I} \otimes \nabla \tilde{v})\mathbf{u})\mathbf{v} - ((\mathbf{I} \otimes \nabla \tilde{v})\mathbf{v})\mathbf{u} = \in \nabla \tilde{v}(\mathbf{u} \times \mathbf{v}). \tag{44}$$

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

$$\hat{\mathbf{p}}^\alpha = \hat{\mathbf{s}}^\alpha \times \hat{\mathbf{m}}^\alpha, \quad \mid \hat{\mathbf{p}}^\alpha \mid = \mid \hat{\mathbf{s}}^\alpha \mid \mid \hat{\mathbf{m}}^\alpha \mid$$

$$\hat{\mathbf{s}}^\alpha = \frac{1}{\mid \hat{\mathbf{m}}^\alpha \mid^2} \hat{\mathbf{m}}^\alpha \times \hat{\mathbf{p}}^\alpha, \quad \mid \hat{\mathbf{m}}^\alpha \mid^2 = \mathbf{m}^\alpha \cdot \mathbf{B}^p \mathbf{m}^\alpha, \quad \mathbf{B}^p = \mathbf{F}^p(\mathbf{F}^p)^T. \tag{45}$$

Remark. 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 (43) with other results in literature, only with regards to the Schmid effect (i.e. when the normal plastic components $\hat{\gamma}^\alpha, \tilde{\gamma}$ are vanishing). 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 [4]. Here we denoted this tensor by $\mathbf{G}^C$ to make difference between them. The plastically convected rate of $\mathbf{G}^C$, see formula (30), has a similar expression as in (43), when $\hat{\mathbf{m}}$ is absent.

3. PRINCIPLE OF THE FREE ENERGY IMBALANCE

3.1. VIRTUAL POWER PRINCIPLE

We exemplify the **the virtual power principle** formulated by Gurtin and Anand [23] for the small strains and the derived macroscopic and microscopic force balances, see also Gurtin et al. [24].

Let $\mathscr{P}$ and $\partial\mathscr{P}$ be an arbitrary part of the body and its boundary, respectively.

Internal power is defined in terms of the elastic and plastic rates, $\dot{\mathbf{E}}^e$ and $\dot{\mathbf{E}}^p$, by

$$\mathscr{W}_{int} = \int_{\mathscr{P}} (\mathbf{T} \cdot \dot{\mathbf{E}}^e + \mathbf{T}^p \cdot \dot{\mathbf{E}}^p + \mathbf{K} \cdot \nabla \dot{\mathbf{E}}^p)\, dV \tag{46}$$

with $\mathbf{T}$ Cauchy stress tensor and $\mathbf{T}^p$ a micro force, which is power conjugate with $\dot{\mathbf{E}}^p$.

The internal power must be balanced by the external power expended by the tractions on ∂P and body forces acting within $\mathscr{P}$, which are supplemented with a higher-order power expenditure involving the so-called *hypertraction* $\mathbf{K}(\mathbf{n})$. The external power has the form

$$\mathscr{W}_{ext} = \int_{\mathscr{P}} \mathbf{b} \cdot \dot{\mathbf{u}}\, dV + \int_{\partial \mathscr{P}} \mathbf{t}(\mathbf{n}) \cdot \dot{\mathbf{u}}\, \mathbf{dA} + \int_{\partial \mathscr{P}} \mathbf{Kn} \cdot \dot{\mathbf{E}}^{\mathbf{p}}\, \mathbf{dV} \tag{47}$$

A *generalized virtual velocity*, $\mathscr{V} = (\tilde{\mathbf{u}}, \tilde{\mathbf{E}}^p, \tilde{\mathbf{E}}^p)$, consistent with the appropriate kinematical relationship $\nabla \tilde{\mathbf{u}} = \tilde{\mathbf{E}}^p + \tilde{\mathbf{E}}^p$, is considerd.

The principle of the virtual power is based on the power balance

$$\mathscr{W}_{ext} = \mathscr{W}_{int}. \tag{48}$$

The expression of the external power contains the term $\mathbf{Kn} \cdot \mathbf{E}^p$, which enters the identity

$$\int_{\mathscr{P}} \mathbf{K} \cdot \nabla \mathbf{E}^p\, dV = -\int_{\mathscr{P}} (Div\mathbf{K}) \cdot \mathbf{E}^p\, dV + \int_{\partial \mathscr{P}} \mathbf{Kn} \cdot \mathbf{E}^p\, dA. \tag{49}$$

- First the principle of the virtual power was formulated.
- The next step is to determine the macro and micro balance equations.

  - The macro balance equation is formulated if $\tilde{\mathbf{u}}$ is arbitrary and $\tilde{\mathbf{E}}^p = 0$. The local macro balance equation and the boundary condition follow

$$\begin{aligned} &div\mathbf{T} + \mathbf{b} = 0, \\ &\mathbf{Tn} = \mathbf{t}(\mathbf{n}) \quad \text{on } \partial \mathscr{P}. \end{aligned} \tag{50}$$

  - The micro balance equation is derived if $\tilde{\mathbf{u}} = 0$ is arbitrary and $\tilde{\mathbf{E}}^e = -\tilde{\mathbf{E}}^p$. The reduced equation is assumed to hold for all $\tilde{\mathbf{E}}^p$. We found that

$$\begin{aligned} &\mathbf{T} = \mathbf{T}^p - Div\mathbf{K}, \\ &\mathbf{Kn} = \mathbf{k}(\mathbf{n}) \quad \text{on } \partial \mathscr{P}. \end{aligned} \tag{51}$$

3.2. LOCAL PRINCIPLE OF THE FREE ENERGY IMBALANCE

Let ψ denotes the free energy density function. The *global free energy principle* requires the variation in time of the free energy do not exceed the expaende external power, namely

$$\frac{d}{dt}\int_{\mathscr{P}} \rho\,\psi\, dV \leq \mathscr{W}_{ext}, \tag{52}$$

As $\mathscr{W}_{ext} = \mathscr{W}_{int}$ the inequality holds

$$\int_{\mathscr{P}} \rho\,\dot{\psi}\, dV \leq \int_{\mathscr{P}} (\mathbf{T}\cdot\dot{\mathbf{E}}^e + \mathbf{T}^p\cdot\dot{\mathbf{E}}^p + \mathbf{K}\cdot\nabla\dot{\mathbf{E}}^p)\, dV. \tag{53}$$

Thus the **local free-energy imbalance** follows

$$\rho\,\dot{\psi} \leq \mathbf{T}\cdot\dot{\mathbf{E}}^e + \mathbf{T}^p\cdot\dot{\mathbf{E}}^p + \mathbf{K}\cdot\nabla\dot{\mathbf{E}}^p. \tag{54}$$

Remark. Since $\mathbf{E}^p$ is dimensionless $\nabla\mathbf{E}^p$ carries dimensions of $length^{-1}$.

Within the finite elasto-plasticity framework we reformulate the local imbalance of the free energy principle as:

AXIOM 3. (The local form of the global principle of the free energy imbalance). *The elasto-plastic behavior of the material is restricted to satisfy, for any virtual (isothermal) process, the free energy imbalance in $\mathscr{K}$, namely*

$$(\mathscr{P}_{int})_{\mathscr{K}} - \dot{\psi}_{\mathscr{K}} \geq 0. \tag{55}$$

Here $(\mathscr{P}_{int})_{\mathscr{K}}$ is the mass density of the internal power and $\psi_{\mathscr{K}}$ is the free energy density in $\mathscr{K}$.

The models are strongly dependent on the expression considered for the free energy function. Further, two possible models, provided by Cleja-Ţigoiu [17], and Cleja-Ţigoiu and Paşcan [13], are presented. We analyze the restrictions on the constitutive equations that follow from the local imbalance free energy principle.

4. MODEL WITH SCALAR DISLOCATION DENSITIES AND NON-SCHMID FLOW RULE

4.1. MODEL WITH SCALAR DISLOCATION DENSITIES

Model **M1:** In order to provide the model with scalar dislocation densities, proposed by Cleja-Ţigoiu [13], we introduce the basic assumptions:

- The free energy density is postulated to be dependent on the elastic strain, $\mathbf{C}^e$, as a measure of the elastic deformation, and on the *scalar dislocation density*, $\rho^d_{\mathscr{K}}$, and its gradient, $\nabla_{\mathscr{K}}\,\rho^d_{\mathscr{K}}$, with respect to the configuration $\mathscr{K}$, i.e.

$$\psi = \psi_{\mathscr{K}}(\mathbf{C}^e, \rho^d_{\mathscr{K}}, \nabla_{\mathscr{K}}\,\rho^d_{\mathscr{K}}), \quad \mathbf{C}^e = (\mathbf{F}^e)^T\mathbf{F}^e. \tag{56}$$

- The expression of the mass density of the internal power, $(\mathscr{P}_{int})_{\mathscr{K}}$, is given by

$$(\mathscr{P}_{int})_{\mathscr{K}} = \frac{1}{2\widetilde{\rho}}\boldsymbol{\pi}\cdot\dot{\mathbf{C}}^e + \frac{1}{\widetilde{\rho}}\mathbf{g}^p\cdot\mathbf{L}^p + \frac{1}{\widetilde{\rho}}g^d\cdot\frac{d}{dt}(\rho^d_{\mathscr{K}}) + \frac{1}{\widetilde{\rho}}\mathbf{m}^d\cdot\frac{d}{dt}(\nabla_{\mathscr{K}}\rho^d{}_{\mathscr{K}}), \tag{57}$$

  where $\boldsymbol{\pi}$ denotes the Piola-Kirchoff stress tensor, and $\mathbf{g}^p$ is the micro force power conjugate to the rate of plastic distortion $\mathbf{L}^p$.

- The micro stress, $g^d \in R$, and micro momentum, $\mathbf{m}^d \in \mathscr{V}$, are related to the dislocation mechanism, being power conjugate to the appropriate rate of dislocation density and its gradient. These micro forces comply the balance equation, which is postulated in the form written below with respect to the reference configuration

$$J^p\, g^d = \operatorname{div}\mathbf{m}^d_0 + \hat{\rho}_0 B^d, \quad \text{where} \quad J^p = \det\mathbf{F}^p = \frac{\hat{\rho}_0}{\widetilde{\rho}}, \tag{58}$$

  where B^d is given, while $\hat{\rho}_0$ is the mass density in the reference configuration. The micro momentum, $\mathbf{m}^d_0$, is defined with respect to the reference configuration, and is related with $\mathbf{m}^d$ through the following relation

$$\mathbf{m}^d = J^p\mathbf{F}^p\mathbf{m}^d_0. \tag{59}$$

- The Piola-Kirchhoff and Cauchy stress tensors, $\boldsymbol{\pi}$ and $\mathbf{T}$, respectively, are related by $\frac{1}{\tilde{\rho}}\boldsymbol{\pi} = (\mathbf{F}^e)^{-1}\frac{1}{\bar{\rho}}\mathbf{T}(\mathbf{F}^e)^{-T}$, where $\tilde{\rho}$ and $\bar{\rho}$ are the mass densities with respect to the isoclinic and actual configurations, respectively.

The expression of the free energy density (56) can be derived in terms of the fields related to the reference configuration by using the pulled back procedure and the formulae written in (8), (14), namely

$$\begin{aligned} &\psi = \psi(\mathbf{C}, \mathbf{F}^p, \rho^d, \nabla\,\rho^d), \\ &\text{since} \quad \mathbf{C}^e = (\mathbf{F}^p)^{-T}\mathbf{C}(\mathbf{F}^p)^{-1}, \quad \mathbf{C} = \mathbf{F}^T\mathbf{F}. \end{aligned} \tag{60}$$

We express the *time derivative of the free energy density* directly in terms of the fields related to the reference configuration from (60), in which the special form of the rate of plastic deformation described in (33). Thus the local form of the free density imbalance (55) becomes

$$
\begin{aligned}
&\frac{1}{\tilde{\rho}}\boldsymbol{\pi}\cdot(\mathbf{F}^e)^T\mathbf{D}\mathbf{F}^e-\frac{1}{\tilde{\rho}}\boldsymbol{\pi}\cdot\mathbf{C}^e\mathbf{L}^p+\frac{1}{\tilde{\rho}}\mathbf{C}^e\boldsymbol{\pi}\cdot\mathbf{L}^p-2\mathbf{F}\partial_{\mathbf{C}}\psi\mathbf{F}^T\cdot\mathbf{D}\\
&+\frac{1}{\hat{\rho}_0}g^d\cdot(\dot{\rho}^d-\rho^d\,\mathrm{tr}\mathbf{L}^p)-\partial_{\rho^d}\psi\,\dot{\rho}^d+\frac{1}{\tilde{\rho}}\mathbf{m}^d\cdot\frac{d}{dt}(\nabla_{\mathscr{K}}\rho^d{}_{\mathscr{K}})-\partial_{\nabla\rho^d}\psi\cdot\nabla\dot{\rho}^d \qquad (61)\\
&-\partial_{\mathbf{F}^p}\psi(\mathbf{F}^p)^T)\cdot\{\sum_{\alpha=1}^{N}\nu^\alpha\,(\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha)+\sum_{\alpha=1}^{N}\hat{\nu}^\alpha\,(\mathbf{m}^\alpha\otimes\mathbf{m}^\alpha)+\tilde{\nu}\,\mathbf{I}\}\geq 0.
\end{aligned}
$$

Here $\mathbf{D}=\{\mathbf{L}\}^{\mathbf{S}}$.

4.2. THERMODYNAMIC RESTRICTIONS

We analyze the restrictions imposed by the inequality (61) that holds for any rate of the deformation $\mathbf{D}$. If we consider that the behaviour remains in the elastic domain, then no evolution of the dislocation density and plastic distortion occurs and, consequently the elastic type constitutive equation is derived. When the elastic type constitutive equation is replaced into the inequality (61), the reduced dissipated inequality follows.

THEOREM [14]. *The thermomechanical restrictions imposed by the principle of the free energy imbalance to the constitutive functions are expressed by:*

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*

$$\frac{1}{\rho}\boldsymbol{\pi}=2\,\partial_{\mathbf{C}^e}\psi_{\mathscr{K}} \quad\Longleftrightarrow\quad \frac{1}{\rho}\mathbf{T}=2\mathbf{F}^e(\partial_{\mathbf{C}^e}\psi_{\mathscr{K}})\mathbf{F}^{eT}. \qquad (62)$$

2. *The reduced dissipation inequality can be represented as*

$$
\begin{aligned}
&\sum_{\alpha=1}^{N}\nu^\alpha\,\mathbf{s}^\alpha\cdot\mathbf{t}_{\mathbf{m}^\alpha}+\sum_{\alpha=1}^{N}\hat{\nu}^\alpha\,\mathbf{m}^\alpha\cdot\mathbf{t}_{\mathbf{m}^\alpha}+\tilde{\nu}\,(\mathrm{tr}\Sigma-\nabla_{\mathscr{K}}\rho^d\cdot\frac{1}{\tilde{\rho}}\mathbf{m}^d)\\
&+\Big(\frac{g^d}{\hat{\rho}_0}-\partial_{\rho^d}\,\psi\Big)\cdot\dot{\rho}^d+\Big(\frac{1}{\hat{\rho}_0}\mathbf{m}_0^d-\partial_{\nabla\rho^d}\,\psi\Big)\cdot\nabla\dot{\rho}^d \qquad (63)\\
&-(\hat{\nu}+3\,\tilde{\nu})\,\frac{1}{J^p}\big(\rho^d\,\Upsilon^d-\nabla\rho^d\cdot\mathbf{m}_0^d\big)\geq 0.
\end{aligned}
$$

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

$$\mathbf{t}_{\mathbf{m}^\alpha} := \boldsymbol{\Sigma}\mathbf{m}^\alpha - (\mathbf{m}^\alpha \cdot \frac{1}{\tilde{\rho}}\mathbf{m}^d)\,\frac{1}{J^p}(\mathbf{F}^p)^{-T}\,\nabla\rho^d, \tag{64}$$

where the Mandel type stress tensor, $\boldsymbol{\Sigma}$, with respect to the isoclinic configuration

$$\frac{1}{\hat{\rho}_0}\boldsymbol{\Sigma} = \mathbf{C}^e\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\pi} = -\partial_{\mathbf{F}^p}\psi(\mathbf{F}^p)^T, \tag{65}$$

4.3. MODEL COMPATIBLE WITH FREE ENERGY IMBALANCE

1. The following internal variables are used herein: the dislocation densities ρ^α and hardening variables (or slip resistances) ζ^α in the $\alpha-$slip system, which are described by appropriate evolution equations.
2. The activation condition for a slip system is defined in terms of the generalized resolved stress as

$$\bar{\tau}_e^\alpha := \mid \mathbf{s}^\alpha \cdot \mathbf{t}_{\mathbf{m}^\alpha} \mid + a \mid \mathbf{m}^\alpha \cdot \mathbf{t}_{\mathbf{m}^\alpha} \mid \tag{66}$$

with a positive.

Let us remark that for $a = 0$ and $\mathbf{m} = 0$ the formula (66 together with (64) is reduced to (21).
3. The viscoplastic function is introduced by

$$\mathscr{F}^\alpha := \bar{\tau}_e^\alpha - \zeta^\alpha(\rho^\alpha), \quad \rho^d = (\rho^\alpha)_{\alpha=1,\dots,N.} \tag{67}$$

4. The *hardening law* (i.e. the elasto-plastic material is assumed to be a hardening one) is expressed either in terms of the dislocation densities according to [3]

$$\zeta^\alpha = \zeta^\alpha\big(\rho^\beta\big), \qquad \beta = 1,\dots,N, \tag{68}$$

or by a certain evolution equation, say for example

$$\dot{\zeta}^\alpha = \sum_{\beta=1}^{N} h^{\alpha\beta}\,|\dot{\gamma}^\beta|, \tag{69}$$

where $h^{\alpha\beta}$ is the hardening matrix, strongly dependent on the dislocation densities.

5. The plastic velocities $\nu, \hat{\nu}^\alpha, \tilde{\nu}^\alpha$ are defined as follows

$$
\begin{aligned}
&\nu^\alpha = \dot{\gamma}^\alpha \operatorname{sign}(\mathbf{s}^\alpha \cdot \mathbf{t}_{\mathbf{m}^\alpha}) \mathscr{H}(\bar{\tau}_e - \zeta(\rho)), \\
&\hat{\nu}^\alpha = \dot{\gamma}^\alpha \operatorname{sign}(\mathbf{m}^\alpha \cdot \mathbf{t}_{\mathbf{m}^\alpha}) \mathscr{H}(\bar{\tau}_e - \zeta(\rho)), \\
&\tilde{\nu} = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \operatorname{sign}(\mathrm{tr}\Sigma - \nabla_{\mathscr{K}} \rho^d \cdot \frac{1}{\tilde{\rho}} \mathbf{m}^d) \mathscr{H}(\bar{\tau}_e - \zeta(\rho)),
\end{aligned}
\tag{70}
$$

Here $\mathscr{H}(\mathscr{F}^\alpha)$ is the Heaviside function composed with the viscoplastic function.
6. The *viscoplastic flow rule* is described by

$$
\dot{\gamma}^\alpha = \dot{\gamma}_0^\alpha \left| \frac{\bar{\tau}_e^\alpha}{\zeta^\alpha} \right|^n, \forall \alpha = 1, \ldots, N. \tag{71}
$$

5. MODEL WITH TENSORIAL DISLOCATION DENSITY AND NON-SCHMID FLOW RULE

We present now the model **M2** with scalar dislocation densities and tensorial dislocation tensor provided by Cleja-Ţigoiu [17].

5.1. MODEL WITH SCALAR AND TENSORIAL DISLOCATION DENSITIES

Model **M2** involves the tensorial dislocation tensor **G**. The time derivative of the tensorial dislocation density **G**, defined by (41), is expressed by (43) and contains $\nabla \nu^\alpha, \nabla \hat{\nu}^\alpha, \nabla \tilde{\nu}$, the gradients of the shear and normal platic velocities, $\nu^\alpha, \hat{\nu}^\alpha, \tilde{\nu}$, which are time derivatives of plastic components in slip systems. These fields $\gamma^\alpha, \hat{\gamma}^\alpha, \tilde{\gamma}$ and their gradients enter the expression of the free energy density and prove the circumstantial dependence on the tensorial dislocation density.

The material behavior is restricted to satisfy in $\mathscr{K}$ the *free energy imbalance postulate* (55), under the following hypotheses, see Cleja-Ţigoiu [17]:

- 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

$$
\psi = \psi_{\mathscr{K}} \equiv \psi(\mathbf{C} - \mathbf{C}^p, \gamma^\alpha, \hat{\gamma}^\alpha, \tilde{\gamma}, \nabla \gamma^\alpha, \nabla \hat{\gamma}^\alpha, \nabla \tilde{\gamma}, \rho^d, \nabla \rho^d), \quad \mathbf{C} = (\mathbf{F})^T \mathbf{F}. \tag{72}
$$

  $\mathbf{C}^e - \mathbf{I} = (\mathbf{F}^p)^{-T}(\mathbf{C} - \mathbf{C}^p)(\mathbf{F}^p)^{-1}$. The presence of the plastic distortion, $\mathbf{F}^p$, and its gradient through $\overset{(\mathrm{p})}{\mathscr{A}}$, is generically represented by $\mathbf{C} - \mathbf{C}^p$, the scalar plastic components and their gradients. The free energy density depends also on the scalar dislocation density and its gradient;

- an appropriate definition for the internal power $(\mathscr{P}_{int})_{\mathscr{K}}$, extended to involve the expended 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;

- the free energy imbalance is postulated for any virtual (isothermic) processes, associated with *kinematics* of the deformation process.

Remark. The expression of the free energy density introduced by (72) is essentially different from (56), due to the normal plastic components and their gradients.

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 ([11]). The *balance equation* for macro stress is reduced to the classical one.

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

$$\begin{aligned}(\mathscr{P}_{int})_{\mathscr{K}} &= \frac{1}{2\tilde{\tilde{\rho}}}\,\boldsymbol{\pi}\cdot\dot{\mathbf{C}}^e + \frac{1}{\tilde{\tilde{\rho}}}\mathbf{g}^p\cdot\mathbf{L}^p + \frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p\cdot\nabla_{\mathscr{K}}\mathbf{L}^p + \\ &+\frac{1}{\tilde{\tilde{\rho}}}g^d\cdot\frac{d}{dt}(\rho^d_{\mathscr{K}}) + \frac{1}{\tilde{\tilde{\rho}}}\mathbf{m}^d\cdot\frac{d}{dt}(\nabla_{\mathscr{K}}\rho^d{}_{\mathscr{K}}).\end{aligned} \tag{73}$$

- $\boldsymbol{\pi}$ is the Piola-Kirchhoff stress tensor related with 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, $(\mathbf{L}^p,\nabla_{\mathscr{K}}\mathbf{L}^p)$, and satisfy the micro balance equation in $\mathscr{K}$

$$\mathbf{g}^p = \mathrm{div}_{\mathscr{K}}\,(\boldsymbol{\mu}^p) + \tilde{\rho}\mathbf{B}^p_m. \tag{74}$$

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

Remark. The gradient of the rate of plastic distortion, $\nabla_{\mathscr{K}}\mathbf{L}^p$, has been considered in the expression of the internal dissipated power (73), in contrast to (57), and consequently the micro stress momenta which is related to the plastic mechanism has been introduced as an appropriate conjugate micro force.

PROPOSITION [11]. *The micro balance equation associated with the plastic mechanism is equivalently written with respect to the reference configuration*

$$J^p\,\mathbf{g}^p = div\,(J^p\boldsymbol{\mu}^p(\mathbf{F}^p)^{-1}) + \hat{\rho}\mathbf{B}^p_m. \tag{75}$$

$\mathbf{B}_m^p$ *mass density of the couple body force, related with the plastic mechanism.*

In order to emphasize the thermodynamic restriction imposed by the principle of the free energy imbalance, the internal power dissipated by the plastic mechanism have to be computed. We use algebraic formulae that hold for second and third order tensor fields

$$
\begin{aligned}
&\mathbf{A}\cdot\mathbf{F}_1\mathbf{B}\mathbf{F}_2 = (\mathbf{F}_1)^T\mathbf{A}(\mathbf{F}_2)^T\cdot\mathbf{B},\\
&\mathscr{A}[\mathbf{F},\mathbf{I}] = \mathscr{A}\mathbf{F},\\
&\mathscr{A}[\mathbf{F}_1,\mathbf{F}_2]\cdot\mathscr{B} = \mathscr{A}\cdot\mathscr{B}[(\mathbf{F}_1)^T,(\mathbf{F}_2)^T],\\
&J^p = \frac{\tilde{\rho}}{\hat{\rho}_0},
\end{aligned}
\tag{76}
$$

Here $\mathbf{A},\mathbf{B},\mathbf{F}_j,\mathbf{F}\in Lin$, and $\mathscr{A},\mathscr{B}\in Lin(\mathscr{V},Lin)$.

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

$$\frac{1}{\tilde{\rho}}\mathbf{g}^p\cdot\mathbf{L}^p = \frac{1}{\hat{\rho}_0}\mathbf{\Sigma}_0^p\cdot\hat{\mathbf{l}}^p, \quad \text{with} \quad \frac{1}{\hat{\rho}_0}\mathbf{\Sigma}_0^p = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^T\mathbf{g}^p(\mathbf{F}^p)^{-T}, \tag{77}$$

as a consequence of the formulae (37) and (76). Here $\mathbf{\Sigma}_0^p$ is the Mandel's stress measure associated with the micro plastic stress $\mathbf{g}^p$.

As a consequence of the formulae (38) and (77) the power delivered by $\mathbf{g}^p$ is given by

$$\sum_{\alpha=1}^{N}\frac{1}{\rho_0}\mathbf{\Sigma}_0^p\cdot(\hat{\mathbf{s}}^\alpha\otimes\hat{\mathbf{m}}^\alpha)\,\nu^\alpha + \sum_{\alpha=1}^{N}\frac{1}{\rho_0}\mathbf{\Sigma}_0^p\cdot((\mathbf{C}^p)^{-1}\hat{\mathbf{m}}^\alpha\otimes\hat{\mathbf{m}}^\alpha)\,\hat{\nu}^\alpha + \tilde{\nu}\,\frac{1}{\rho_0}\mathbf{\Sigma}_0^p\cdot\mathbf{I} \tag{78}$$

In order to express the power expanded by the plastic micro momentum we use the algebraic formulae (76) and we proceed as follows:

- First we recall the formula which gives the gradient, $\nabla_{\mathscr{K}}\mathbf{L}^p$ in terms of the time derivative of $\overset{(p)}{\mathscr{A}}$, and second we replace the time derivative of $\overset{(p)}{\mathscr{A}}$ through the expression (40), and finally it results

$$\begin{aligned}\nabla_{\mathscr{K}}\mathbf{L}^p = \mathbf{F}^p\frac{d}{dt}(\overset{(\mathrm{p})}{\mathscr{A}})[(\mathbf{F}^p)^{-1},(\mathbf{F}^p)^{-1}] = \sum_{\alpha=1}^{N}\{\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\nu^\alpha\}[(\mathbf{F}^p)^{-1},\mathbf{I}]+ \\ +\sum_{\alpha=1}^{N}\{\mathbf{m}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\hat{\nu}^\alpha\}[\mathbf{F}^p)^{-1},\mathbf{I}]+(\mathbf{I}\otimes\nabla\tilde{\nu})[(\mathbf{F}^p)^{-1},\mathbf{I}]\end{aligned} \tag{79}$$

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

$$\begin{aligned}\nabla_{\mathscr{K}}\mathbf{L}^p\cdot\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p = \sum_{\alpha=1}^{N}\{\mathbf{s}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\nu^\alpha\}\cdot\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T}+ \\ +\sum_{\alpha=1}^{N}\{\mathbf{m}^\alpha\otimes\mathbf{m}^\alpha\otimes\nabla\hat{\nu}^\alpha\}\cdot\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T}+(\mathbf{I}\otimes\nabla\tilde{\nu})\cdot\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T}.\end{aligned} \tag{80}$$

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

$$\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p := (\mathbf{F}^p)^T\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p[(\mathbf{F}^p)^{-T},(\mathbf{F}^p)^{-T}]. \tag{81}$$

Consequently, the mechanical power dissipated by the micro plastic momentum given in (80) can be rewritten as

$$\begin{aligned}\nabla_{\mathscr{K}}\mathbf{L}^p\cdot\frac{1}{\tilde{\tilde{\rho}}}\boldsymbol{\mu}^p = \sum_{\alpha=1}^{N}\{\hat{\mathbf{s}}^\alpha\otimes\hat{\mathbf{m}}^\alpha\}\cdot(\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T}\nabla\nu^\alpha)+ \\ +\sum_{\alpha=1}^{N}(\mathbf{C}^p)^{-1}\{\hat{\mathbf{m}}^\alpha\otimes\hat{\mathbf{m}}^\alpha\}\cdot\frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p((\mathbf{F}^p)^{-T}\nabla\hat{\nu}^\alpha)+\mathbf{I}\cdot\frac{1}{\hat{\rho}}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T}\nabla\tilde{\nu}).\end{aligned} \tag{82}$$

when the fields are pulled back to the reference configuration.

- The mechanical power dissipated by the micro stress momentum associated with dislocations, i.e. defined by the last term in (73) is calculated as follows:

We use the relationships between the micro momenta (59), the rate of the gradient of the dislocation density (15), as well as expressions of the rate of the plastic distortion (38) together with (37) and we obtain

$$
\begin{aligned}
&-\frac{1}{\tilde{\tilde{\rho}}}\mathbf{m}^d \cdot \frac{1}{J^p}((\mathbf{F}^p)^{-1}\mathbf{L}^p)^T\, \nabla\rho^d = -\sum_{\alpha=1}^{N} v^\alpha\,(\nabla\rho^d \cdot \hat{\mathbf{s}}^\alpha)(\hat{\mathbf{m}}^\alpha \cdot \frac{1}{\hat{\rho}_0}\mathbf{m}_0^d) +\\
&-\sum_{\alpha=1}^{N} \hat{v}^\alpha\,(\nabla\rho^d \cdot (\mathbf{C}^p)^{-1}\hat{\mathbf{m}}^\alpha)(\hat{\mathbf{m}}^\alpha \cdot \frac{1}{\hat{\rho}_0}\mathbf{m}_0^d) - \tilde{v}\,\nabla\rho^d \cdot \frac{\mathbf{m}_0^d}{\hat{\rho}_0}.
\end{aligned}
\tag{83}
$$

We use again the relationships between the micro momenta (59) and the continuity condition of the mass, namely $\tilde{\rho}\, J^p = \hat{\rho}_0$. We obtain the following representation

$$
\begin{aligned}
&\frac{1}{\tilde{\tilde{\rho}}}\mathbf{m}^d \cdot \frac{1}{J^p}(\mathbf{F}^p)^{-T}\, \nabla\dot{\rho}^d = \frac{1}{\hat{\rho}_0}\,\mathbf{m}_0^d . \nabla\dot{\rho}^d,\\
&-\frac{1}{\tilde{\tilde{\rho}}}\mathbf{m}^d \cdot tr\mathbf{L}^p(\mathbf{F}^p)^{-T}\, \nabla\rho^d = -\frac{1}{\hat{\rho}_0}\,\mathbf{m}_0^d(\hat{v} + 3\tilde{v})\nabla\rho^d.
\end{aligned}
\tag{84}
$$

Finally, the mechanical power dissipated by the micro stress momentum, $\mathbf{m}^d$ can be expressed, see for instance [13].

5.2. ELASTIC-VISCOPLASTIC NON-LOCAL EQUATIONS COMPATIBLE WITH FREE ENERGY IMBALANCE PRINCIPLE

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

$$
\begin{aligned}
&\mathbf{t}_{\hat{\mathbf{m}}^\alpha} := \mathbf{\Sigma}_0^p \hat{\mathbf{m}}^\alpha - (\hat{\mathbf{m}}^\alpha \cdot \mathbf{m}_0^d)\,\nabla\rho^d,\\
&t_{\mathbf{m}^0} = \mathbf{\Sigma}_0^p \cdot \mathbf{I} - \mathbf{m}_0^d \cdot \nabla\rho^d.
\end{aligned}
\tag{85}
$$

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

THEOREM [16]. *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*

$$
\frac{1}{\tilde{\rho}}\boldsymbol{\pi} = 2\,\partial_{\mathbf{C}^e}\psi_{\mathscr{K}} \quad \Longleftrightarrow \quad \frac{1}{\hat{\rho}}\mathbf{T} = 2\mathbf{F}^e(\partial_{\mathbf{C}^e}\psi_{\mathscr{K}})\mathbf{F}^{eT}. \tag{86}
$$

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

2. *The dissipation inequality with respect to the reference configuration for the model* **M2** *yields*

$$
\begin{aligned}
&(\frac{1}{\hat{\rho}_0} g^d - \partial_{\rho^d}\psi) \cdot \dot{\rho}^d + (\frac{1}{\hat{\rho}_0}\mathbf{m}_0^d - \partial_{\nabla\rho^d}\ \psi) \cdot \nabla\dot{\rho}^d - \\
&-\frac{1}{\hat{\rho}_0}(g^d \rho^d + \mathbf{m}_0^d \cdot \nabla\rho^d)(\sum_{\alpha=1}^{N} \hat{\nu^\alpha} + 3\tilde{\nu}^\alpha) + (\frac{1}{\hat{\rho}_0} t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}}\psi)\tilde{\nu} + \\
&+ \sum_{\alpha=1}^{N} (\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi)\nu^\alpha + \sum_{\alpha=1}^{N} (\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot (\mathbf{C}^p)^{-1}\hat{\mathbf{m}}^\alpha - \partial_{\hat{\gamma}^\alpha}\psi)\hat{\nu}^\alpha + \\
&+ \sum_{\alpha=1}^{N} \{(\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\gamma^\alpha}\psi\} \cdot \nabla\nu^\alpha + \\
&+ \sum_{\alpha=1}^{N} \{(\mathbf{C}^p)^{-1}(\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\hat{\gamma}^\alpha}\psi\} \cdot \nabla\hat{\nu}^\alpha \\
&+(\mathbf{I} : \frac{1}{\hat{\rho}_0}\boldsymbol{\mu}_0^p(\mathbf{F}^p)^{-T} - \partial_{\nabla\tilde{\gamma}}\psi) \cdot \nabla\tilde{\nu} \geq 0.
\end{aligned}
\tag{87}
$$

The micro forces $(g^d, \mathbf{m}^d)$ are related to the dislocation mechanism and satisfy the micro balance equation given by (58) together with (59).

In order **to simplify the constitutive relationships** the following **energetic constitutive equations** can be introduced, if we adopt the method proposed by Grudmundson [21].

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

$$
\frac{1}{\hat{\rho}_0}\mathbf{m}_0^d - \partial_{\nabla\rho^d}\ \psi = 0. \tag{88}
$$

Let $\mathscr{P}_t$ be the plastically deformed domain at a fixed moment of time. If we assume that the micro momentum associated with the microbalance equation (58) on the boundary $\partial\mathscr{P}_t$ 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 $g^d\rho^d + \mathbf{m}_0^d \cdot \nabla\rho^d$, i.e.
$\int_{\partial\mathscr{P}_t} (g^d\rho^d + \mathbf{m}_0^d \cdot \nabla\rho^d) dV = 0$, becomes zero due to the micro balance equation. This is the rationale to eliminate the third term in (87).

• 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

$$
\begin{aligned}
&(\hat{\mathbf{s}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0} \boldsymbol{\mu}_0^p (\mathbf{F}^p)^{-T} - \partial_{\nabla \gamma^\alpha} \psi = 0 \\
&(\mathbf{C}^p)^{-1} (\hat{\mathbf{m}}^\alpha \otimes \hat{\mathbf{m}}^\alpha) : \frac{1}{\hat{\rho}_0} \boldsymbol{\mu}_0^p (\mathbf{F}^p)^{-T} - \partial_{\nabla \hat{\gamma}^\alpha} \psi = 0 \\
&\mathbf{I} : \frac{1}{\hat{\rho}_0} \boldsymbol{\mu}_0^p (\mathbf{F}^p)^{-T} - \partial_{\nabla \tilde{\gamma}} \psi = 0
\end{aligned}
\tag{89}
$$

The lattice vectors with respect to the reference configuration do not have the unit length and therefore we use the equivalent formulae associated with (89), but relative to the lattice configuration.

PROPOSITION. *The plastic micro momentum which satisfied the restriction written in the above formulae*

$$
\begin{aligned}
\frac{1}{\tilde{\rho}} \boldsymbol{\mu}^p \quad &= \sum_{\alpha=1}^N \big(\mathbf{s}^\alpha \otimes \mathbf{m}^\alpha\big) \otimes \mathbf{F}^p \ (\partial_{\nabla \gamma^\alpha} \psi) + \\
&+ \sum_{\alpha=1}^N \big(\mathbf{m}^\alpha \otimes \mathbf{m}^\alpha\big) \otimes \mathbf{F}^p \ (\partial_{\nabla \hat{\gamma}^\alpha} \psi) + \mathbf{I} \otimes \mathbf{F}^p \ (\partial_{\nabla \tilde{\gamma}} \psi)
\end{aligned}
\tag{90}
$$

The dissipation inequality (87) is then reduced to

$$
\begin{aligned}
&(\frac{1}{\hat{\rho}_0} g^d - \partial_{\rho^d} \psi) \cdot \dot{\rho}^d + (\frac{1}{\hat{\rho}_0} t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}} \psi) \tilde{\nu} + \\
&+ \sum_{\alpha=1}^N (\frac{1}{\hat{\rho}_0} \mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha} \psi) \nu^\alpha + \sum_{\alpha=1}^N (\frac{1}{\hat{\rho}_0} \mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{m}}^\alpha - \partial_{\hat{\gamma}^\alpha} \psi) \hat{\nu}^\alpha \geq 0.
\end{aligned}
\tag{91}
$$

Consequently, the elastic type constitutive equation is given by (86), the energetic representation for the micro momenta are written in (88) and (89).

Remark. We emphasize here evolution equations, for the dislocation density and components of rate of plastic distortion derived following the representation proposed in Gurtin and Anand [23] and given by Cleja-Ţigoiu [17].

1. The evolution equation for the dislocation density will be taken in the form

suggested by the dissipated power

$$\dot{\rho}^d = \beta_1 \big(\frac{g^d}{\hat{\rho}_0} - \partial_{\rho^d}\, \psi\big), \tag{92}$$

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

$$\begin{aligned} \xi^{\alpha}\, \nu^{\alpha} \quad &= \big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{s}}^{\alpha} - \partial_{\gamma^\alpha} \psi\big) \\ \hat{\xi}^{\alpha}\, \hat{\nu}^{\alpha} \quad &= \big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{m}}^{\alpha} - \partial_{\hat{\gamma}^\alpha} \psi\big) \\ \tilde{\xi}\; \tilde{\nu} \quad &= \big(\frac{1}{\hat{\rho}_0} t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}} \psi\big). \end{aligned} \tag{93}$$

and the equivalent plastic rate

$$\lambda^{\alpha} = \sqrt{(\nu^{\alpha})^2 + (\hat{\nu}^{\alpha})^2 + \frac{1}{N^2}\,(\tilde{\nu})^2} \tag{94}$$

3. The equivalent stress measure for $\alpha-$ slip system can be introduced

$$\tau^{\alpha} = \sqrt{\big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{s}}^{\alpha} - \partial_{\gamma^\alpha} \psi\big)^2 + \big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{m}}^{\alpha} - \partial_{\hat{\gamma}^\alpha} \psi\big)^2 + \frac{1}{N^2}\big(\frac{1}{\hat{\rho}_0} t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}} \psi\big)^2} \tag{95}$$

4. We assume that the functions $\xi^{\alpha}, \hat{\xi}^{\alpha}, \tilde{\xi}$ take values, which are proportional with $(\frac{\lambda^{\alpha}}{\lambda_0^{\alpha}})^m$, i.e.

$$\begin{aligned} \big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{s}}^{\alpha} - \partial_{\gamma^\alpha} \psi\big) \quad &= \nu^{\alpha} S_Y\, (\frac{\lambda^{\alpha}}{\lambda_0^{\alpha}})^m \\ \big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha} \cdot \hat{\mathbf{m}}^{\alpha} - \partial_{\hat{\gamma}^\alpha} \psi\big) \quad &= \hat{\nu}^{\alpha} S_Y (\frac{\lambda^{\alpha}}{\lambda_0^{\alpha}})^m \\ \big(\frac{1}{\hat{\rho}_0} t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}} \psi\big) \quad &= \tilde{\nu} S_Y (\frac{\lambda^{\alpha}}{\lambda_0^{\alpha}})^m. \end{aligned} \tag{96}$$

As a direct consequence of the constitutive relationships (95) and (96) the following equality holds

$$(\tau^\alpha)^2 = S_Y^2 \, (\lambda_0^\alpha)^2 (\frac{\lambda^\alpha}{\lambda_0^\alpha})^{2(m+1)}, \text{or equivalently} \quad \frac{\lambda_0^\alpha}{\lambda^\alpha} = (\frac{\tau^\alpha}{S_Y\, \lambda_0^\alpha})^{\dfrac{1}{m+1}}. \tag{97}$$

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

$$\begin{aligned}
v^\alpha &= \frac{\lambda_0^\alpha}{\lambda^\alpha}\big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot \hat{\mathbf{s}}^\alpha - \partial_{\gamma^\alpha}\psi\big)\mathscr{H}(\tau^\alpha - \zeta^\alpha)\\
\hat{v}^\alpha &= \frac{\lambda_0^\alpha}{\lambda^\alpha}\big(\frac{1}{\hat{\rho}_0}\mathbf{t}_{\hat{\mathbf{m}}^\alpha}\cdot \hat{\mathbf{m}}^\alpha - \partial_{\hat{\gamma}^\alpha}\psi\big)\mathscr{H}(\tau^\alpha - \zeta^\alpha)\\
\tilde{v} &= \frac{\lambda_0^\alpha}{\lambda^\alpha}\big(\frac{1}{\hat{\rho}_0}t_{\mathbf{m}^0} - \partial_{\tilde{\gamma}}\psi\big)\mathscr{H}(\tau^\alpha - \zeta^\alpha),
\end{aligned} \tag{98}$$

with $\dfrac{\lambda_0^\alpha}{\lambda^\alpha}$ expressed in terms of the stress by $(97)_2$, and the evolution equation for the dislocation density has been written in (92).

Conclusion. We analyze the description of the proposed model:

- elastic type constitutive equation, from (86);
- viscoplastic constitutive relations written in (98) together with (97) and (56), where $\mathbf{t}_{\hat{\mathbf{m}}^\alpha}$ and $\mathbf{t}_{\mathbf{m}_0}$ are defined in (85) in terms of $\mathbf{\Sigma}_0^p\hat{\mathbf{m}}^\alpha$ and $\mathbf{m}_0^d$;
- the Mandel type stress measure $\mathbf{\Sigma}_0^p$ related to plastic behaviour is given by the relationships (77) together with (74), namely

$$\frac{1}{\hat{\rho}_0}\mathbf{\Sigma}_0^p = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^T \text{ div } (J^p\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T})(\mathbf{F}^p)^{-T}, \tag{99}$$

  while $J^p\boldsymbol{\mu}^p(\mathbf{F}^p)^{-T}$ is described by an energetic relationship given by (90).

- $\mathbf{m}_0^d$ is given by (88), $\dfrac{1}{\hat{\rho}_0}\mathbf{m}_0^d - \partial_{\nabla\rho^d}\,\psi = 0.$
- Finally the evolution equation for the hardening parameters ζ^α (as for instance in Teodosiu and Sidoroff [34]), which enter the expression of viscoplastic equations (98) through the activation function.

- The non local evolution for the scalar dislocation density is defined by (92), together (88) and (58)

$$\dot{\rho}^d = \beta_1 \left(\frac{1}{\tilde{\rho}} \mathrm{div}\, \partial_{\nabla\rho^d}\, \psi - \partial_{\rho^d}\, \psi\right) \tag{100}$$

7. CONCLUSIONS

The rate type constitutive model described above with non-Schmid flow rule and compatible with the principle of the free energy density imbalance can be seen as a generalization of the viscoplastic model developed by Teodosiu and Sidoroff [34]. Our statements is based on the facts that if

• a=0 (which means that the generalized resolved stress defined in (66) is not influenced by the normal direction to the slip system),

• the rate of plastic strain is compatible with plastic incompressibility, i.e. $tr\mathbf{L}^p = 0$, and

• $\mathbf{m}^d = 0$, which means that the micro stress momentum associated with the dislocation mechanism is vanishing, then the formulae (20)-(23) together with (26) follow.

We compare the generalized stress vectors introduced by (64) and (85), related to the models **M1** and **M2**, respectively. These two vectors are defined with respect to the lattice and initial configurations, respectively. The generalized stress vectors (85) are dependent on Mandel's stress measure with respect to the plastically deformed configuration, $\mathbf{\Sigma}_0^p$, which is expressed by $\boldsymbol{\mu}^p$, see the formulae (99) and (90).

The generalized stress vectors (64) are dependent on Mandel's stress measure with respect to the reference configuration, $\mathbf{\Sigma}$, which is expressed in terms of Piola-Kirchoff stress tensor with respect to the reference configuration. Consequently the plastic velocities are completely different in the considered models.

The non-local, dissipative equations can be associated with the model **M1** to characterize the evolution in time of scalar dislocation densities ρ^α. If the following set of constitutive relations are considered

$$\begin{aligned} &\dot{\rho}^d = \beta_1 \left(\frac{g^d}{\hat{\rho}_0} - \partial_{\rho^d}\, \psi\right) \\ &\frac{1}{\hat{\rho}_0}\mathbf{m}_0^d = \partial_{\nabla\rho^d}\, \psi, \quad \partial_{\nabla\rho^d}\, \psi = \kappa_2\, \nabla\rho^d, \end{aligned} \tag{101}$$

together with the micro balance equation (58), then a *non-local evolution equation* *for the scalar dislocation density* yields

$$\dot{\rho}^d = \beta_1 \left(\operatorname{div}\left(\kappa_2 \, \nabla\rho^d\right) - \partial_{\rho^d} \, \psi_T \right). \tag{102}$$

The evolution equation for the scalar dislocation densities are similar in the considered models, as this can be seen by comparing equations (92) and (101).

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