

Different approaches to model the structural defects in elasto-plasticity

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Abstract - The paper deals with macroscopic elasto-plastic models able to describe the material behaviour of the crystalline body containing defects at the microstructural level (structural defects), such as dislocations and disclinations. Within the finite elasto-plasticity the defects will be presented in the so-called plastically deformed configurations, which are embedded with a non-Riemannian geometric structure, characterized by the plastic distortion and the so-called plastic connection. There are presented different, independent ways from the geometrical point of view in defining the two types of defects, which lead to completely different mathematical descriptions or theories. The presence of the Burgers and Frank vectors is the starting point in constructing the dislocation and disclination models. The consequences that follow from the finite elasto-plastic deformations, when the small elastic and plastic distortions are small, are compared with the incompatibilities in small deformation elasto-plasticity. The energetic arguments are analyzed to show how the structural defects can be incorporated into the models.

Key words and phrases : elasto-plasticity, finite deformations, dislocations, disclinations, plastic distortion, plastic connection, energy imbalance principle, constitutive restrictions, evolution equations.

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1. Introduction

The papers deals with macroscopic elasto-plastic models able to describe the material behaviour of the crystalline body containing defects at the microstructural level (structural defects), such as dislocations and disclinations. Within the finite elasto-plasticity the defects will be presented in the so-called plastically deformed configurations, which are embedded with a non-Riemannian geometric structure, characterized by the plastic distortion and the so-called plastic connection. The defects such as dislocations and disclinations are characterized (from physically point of view) by the presence of zones with supplementary atoms and by their geometrical measure in terms of the torsion and curvature of the so-called plastic connection - see de Wit [17], Kröner [26], [27], Cleja-Țigoiu [7], [8], [9]. The point defects (see Kröner [26]), which means extra-matter or voids from the physical point of view, have been characterized from the geometrical point of view in terms

of the non-metric property of the plastic connection and are not considered here. Such type of defects have been included for instance in the paper by Cleja-Țigoiu and V. Țigoiu in [10]. In [14], within the small deformation framework, de Wit provided that is not possible to have *a disclinations theory without dislocations*, but a *pure dislocations theory* can be constructed. The presence of the Burgers and Frank vectors is the starting point in constructing the dislocations and disclinations models - see Gurtin [21], [22]. Under the constitutive relationships the geometric aspects of the deformability of materials with microstructural defects are related with the forces (i.e. with the statics) and the balance equations for forces lead to initial and boundary value problems, which complete the models - see Acharya [2] and Gurtin et al., [22].

Material properties of the metals are strongly influenced by the microstructural and substructural changes during the deformation processes, operating on the structural (micro scale) as well as the substructural (sub-micro scale). The scale level in the deformed material is classified as atomic scale in the range of 1 to 10 nanometer, dislocation scale from 0.1 to 1 micron, grain scale from 1 to 100 μm , and macro scale if the size is greater than 100 μm .

From the historical point of view, Volterra (1909), [46], was the first who introduced lattice defects related to their *translational and rotational* motions, called *distortions*. Disclinations, as a second species of deformation carrying defects, are especially adapted to rotational modes and to the mesoscopic and structural levels, unlike the dislocations, which are especially adapted to translational modes and to the microstructure. The dislocations as well as the disclinations have been illustrated similarly with the help of a Volterra process: an elastic hollow cylinder is cut by a median plane, the two shores of the cut are rotated (disclinations) instead of the translated (dislocations) relative to each other. The strength of dislocation is determined by Burgers vector \mathbf{b} , which is equal to the translational displacement of the non-deformed surfaces of the cut bounded by a dislocation line. In a similar way, the strength of disclination is related to an axial vector $\mathbf{\Omega}$ (Frank vector), which defines the mutual rotation of the undeformed surfaces of the cut bounded by a disclination line.

There are different, independent ways from the geometrical point of view in defining the two types of defects, which include dislocations and disclinations, namely by considering the discrete lines of defects, continuous distributions of the defects, or continuous distribution of infinitesimal loops, which may or may not be related to each other, and which lead to completely different mathematical descriptions or theories. Nabarro [32], was the first who paid attention to the disclinations, as physical objects, as a special and strong source of internal energy which is very large in comparison to the energy of standard dislocations.

The transmission electron microscopy put into evidence the occurrence of self organized structures, ladder like structure or persistent slip bands which evolve, and provides measurements of wavelengths and of the dislocations and disclinations **global average densities** - see for instance references in [39]. The physical examples of rotational defect structures, related with disclinations and which can be observed in crystalline materials are presented by Romanov in [38]. The properties of the disclinations are also discussed as well as disclinations models are developed to explain the physical and mechanical properties of materials. Romanov and Kolesnikova, see [39] proposed that the diffraction contrast observed in the transmission electron microscopy to be associated with the elastic distortion of the crystalline lattice caused by disclinations. The evolution of the **dislocation-disclination ensemble** is described by Romanov [38], Romanov and Kolesnikova [39], Walgraef and Aifantis [47], [49], Seefeldt and Klimanek [40], [41] and Seefeldt et al. [42]. The evolution equations in terms of the densities of dislocations and disclinations, denoted by ρ and θ can be found in [38], as follows

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= F(\rho) - L(\theta)B\rho^2 - M\rho\theta + D\frac{\partial^2 \rho}{\partial x^2}, \\ \frac{\partial \theta}{\partial t} &= -Q(\theta) + \mu M\rho\theta.\end{aligned}\tag{1.1}$$

$F(\rho)$ is the source term for dislocations, $L(\theta)$ reflects the role of the disclinations on the process of annihilation, interactions of disclinations with dislocations lead to a decrease of the dislocation density ρ with the rate $M\rho\theta$ and to the formation of disclination defects (with $\mu \ll 1$). The mobility of dislocations is described with the aid of diffusion-like term, with D the diffusion like coefficient. The parameters which enter the evolution equations have to be determined from microscopic considerations.

The aims of the researches in the mentioned direction are motivated to schematize the essential microstructural features of the deformed single crystals and to connect the above mentioned defects to yield stress contributions.

There are four main structural levels which are dealt with the physics of plasticity, a microscopic level - the scale of the lattice constant, a mesoscopic level - the scale of dislocation substructure, a structural level - the scale of grains in polycrystals, a macroscopic level - the scale of an average physical and mechanical properties. The mesoscopic level (of dislocations) can be characterized by $l_{meso} = \frac{Gb}{\sigma_l}$, where G is the elastic shear modulus, b is the magnitude of lattice dislocation Burgers vector, σ_l is the resistance to motion of an individual dislocation. Generally $l_{meso} \in [0.1\mu m, 1.0\mu m]$.

In the present paper, after a short introduction, the incompatibilities in classical elasticity are presented within the small deformation formalism, the

consequences that follow from the finite elasto-plastic deformations when the small elastic and plastic distortions are considered, the different approaches to structural defects like dislocations and disclinations are analyzed and finally the characteristic features of the model with configuration with torsion (namely an anholonomic configuration, see [1]) is presented to show how the structural defects can be incorporated into the models.

Further the following notations will be used:

- *Lin* – the set of the linear mappings from the vector space \mathcal{V} to \mathcal{V} , i.e the set of second order tensor; $\mathbf{u} \cdot \mathbf{v}$, $\mathbf{u} \times \mathbf{v}$, $\mathbf{u} \otimes \mathbf{v}$ denote scalar, cross and tensorial products of vectors; $(\mathbf{u}, \mathbf{v}, \mathbf{z}) := (\mathbf{u} \times \mathbf{v}) \cdot \mathbf{z}$ is the mixt product of the vectors from \mathcal{V} ; $\mathbf{a} \otimes \mathbf{b}$ and $\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}$ are defined to be a second order tensor and a third order tensor by - $(\mathbf{a} \otimes \mathbf{b})\mathbf{u} = \mathbf{a}(\mathbf{b} \cdot \mathbf{u})$, and $(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c})\mathbf{u} = (\mathbf{a} \otimes \mathbf{b})(\mathbf{c} \cdot \mathbf{u})$, respectively, for all vectors \mathbf{u} . For $\mathbf{A} \in \text{Lin}$ - a second order tensor -, we denote $\{\mathbf{A}\}^S, \{\mathbf{A}\}^a$ for the symmetric and skew-symmetric parts of \mathbf{A} . \mathbf{I} is the identity tensor in *Lin*, \mathbf{A}^T denotes the transpose of $\mathbf{A} \in \text{Lin}$. We mention also the definition for the trace: $\text{tr}\mathbf{A}((\mathbf{u} \times \mathbf{v}) \cdot \mathbf{z}) = (\mathbf{A}\mathbf{u}, \mathbf{v}, \mathbf{z}) + (\mathbf{u}, \mathbf{A}\mathbf{v}, \mathbf{z}) + (\mathbf{u}, \mathbf{v}, \mathbf{A}\mathbf{z})$ and for the tensorial product $\mathbf{A} \otimes \mathbf{a}$ for $\mathbf{a} \in \mathcal{V}$, viewed as a third order tensor given by: $(\mathbf{A} \otimes \mathbf{a})\mathbf{v} = \mathbf{A}(\mathbf{a} \cdot \mathbf{v}), \forall \mathbf{v} \in \mathcal{V}$. $\partial_{\mathbf{A}}\phi(x)$ denotes the partial differential of the function ϕ with respect to the field \mathbf{A} .
- For the differential operators we use: *Curl* of a second order tensor field \mathbf{A} as a second order tensor field defined

$$(\text{curl}\mathbf{A})(\mathbf{u} \times \mathbf{v}) := (\nabla\mathbf{A}(\mathbf{u}))\mathbf{v} - (\nabla\mathbf{A}(\mathbf{v}))\mathbf{u}, \quad \forall \mathbf{u}, \mathbf{v} \in \mathcal{V} \quad (1.2)$$

We remark that $(\text{curl}\mathbf{A})_{pi} = \epsilon_{ijk} \frac{\partial A_{pk}}{\partial x^j}$ are the components of *curl* \mathbf{A} given in a Cartesian basis. $\nabla\mathbf{A}$ is the differential (or the gradient) of the field \mathbf{A} , in a coordinate system $\{\mathbf{x}^a\}$ (with respect to the reference configuration), $\nabla\mathbf{A} = \frac{\partial A_{ij}}{\partial x^k} \mathbf{e}^i \otimes \mathbf{e}^j \otimes \mathbf{e}^k$. 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 $\mathbf{e}^b \cdot \mathbf{e}_a = \delta^b_a$. We use the notation for a third order field $\mathbf{\Gamma}[\mathbf{F}^p, \mathbf{F}^p]$, associated with any second order field \mathbf{F}^p , and third order tensor field $\mathbf{\Gamma}$

$$((\mathbf{\Gamma}[\mathbf{F}^p, \mathbf{F}^p])\mathbf{u})\mathbf{v} = (\mathbf{\Gamma}(\mathbf{F}^p\mathbf{u}))\mathbf{F}^p\mathbf{v}, \quad (1.3)$$

2. Modeling the structural inhomogeneities in finite elasto-plasticity

The *plastic deformability of metals*, which are crystalline materials, is produced due to the *existence of lattice defects inside the microstructure*. Crystalline materials behave like *an elastic body*, either if there are not lattice defects, or if the forces acting on the body are not sufficiently large to move these defects. The lattice defects, among which the *dislocations*, *disclinations* and *point defects* were mathematically modeled by the *differential*

geometry concepts, as torsion, curvature and measure of non-metricity - see Kröner [27] and Noll [37]. The linear approximation of the continuum theory of lattice defects within the non-Euclidean geometry has been proposed by de Wit [17].

We provide now the fundamental concepts related to the model of the materials which contain defects, as a combination of dislocations and disclinations, inside the microstructure, as it can be derived within the second order finite elasto-plasticity, following the papers by Cleja-Tigoiu [7], [8], [9].

As a first step we recall the classical results concerning the integrability theorems (in the smooth case).

Theorem 2.1. (First Integrability Theorem.) *Let \mathcal{U} be a simply connected domain in R^3 and $\mathbf{F} : \mathcal{U} \rightarrow Lin$. The following three assertions are equivalent*

- a. \mathbf{F} is a gradient ,
- b. $(\nabla \mathbf{F}(\mathbf{x})(\mathbf{u}))\mathbf{v} - (\nabla \mathbf{F}(\mathbf{x})\mathbf{v})\mathbf{u} = 0, \quad \forall \mathbf{x} \in \mathcal{U}, \forall \mathbf{u}, \mathbf{v} \in \mathcal{V} \quad (2.1)$
- c. $(curl \mathbf{F}(\mathbf{x}))(\mathbf{u} \times \mathbf{v}) = \mathbf{0}, \quad \forall \mathbf{x} \in \mathcal{U}, \forall \mathbf{u}, \mathbf{v}.$

Definition 2.1. *A connection Γ is integrable if there exists a tensor field \mathbf{F} such that the partial differential equation (written in a local representation) is satisfied*

$$\Gamma = \mathbf{F}^{-1} \nabla \mathbf{F}, \quad \forall \mathbf{x} \in \mathcal{U}, \quad (2.2)$$

Definition 2.2. *The fourth order Riemann-curvature tensor \mathcal{R} , attached to Γ , is defined by*

$$\mathcal{R}(\mathbf{u}, \mathbf{v}) = ((\nabla \Gamma)\mathbf{u})\mathbf{v} - ((\nabla \Gamma)\mathbf{v})\mathbf{u} + (\Gamma\mathbf{u})(\Gamma\mathbf{v}) - (\Gamma\mathbf{v})(\Gamma\mathbf{u}). \quad (2.3)$$

The equation written in definition (2.2) is known as the **second integrability condition**. The following theorem states a relationship between the two definitions.

Theorem 2.2. *The second integrability condition takes place if the Riemann-curvature tensor \mathcal{R} belonging to Γ is vanishing, which means the Frobenius condition holds.*

The models for elasto-plastic materials with structural defects are developed within the constitutive framework of continuum mechanics, using general concepts given by Noll [37], Truesdell and Noll [45], see also Marsden and Hughes [31].

Let us introduce the macro balance equations in the deformed configuration, in forms that contain not only the Cauchy stress, but also the higher

order stresses, as the so-called macro-momentum, following Fleck et al. [18], namely

1. balance of the linear momentum

$$\int_{\chi(\mathcal{P},t)} \hat{\rho} \mathbf{a} dV = \int_{\chi(\mathcal{P},t)} \hat{\rho} \mathbf{b} dV + \int_{\partial\chi(\mathcal{P},t)} \mathbf{t}(\mathbf{n}) dA. \quad (2.4)$$

2. balance of the angular momentum

$$\begin{aligned} \int_{\chi(\mathcal{P},t)} \mathbf{r} \wedge \rho \mathbf{a} dV &= \int_{\chi(\mathcal{P},t)} \mathbf{r} \wedge \rho \mathbf{b} dV + \int_{\partial\chi(\mathcal{P},t)} \mathbf{r} \wedge \mathbf{t}(\mathbf{n}) dA + \\ &+ \int_{\chi(\mathcal{P},t)} \hat{\rho} \mathbf{B}_m dV + \int_{\partial\chi(\mathcal{P},t)} \mathbf{M}(\mathbf{n}) dA, \end{aligned} \quad (2.5)$$

where χ is the motion of the body, $\hat{\rho}$ is the mass density in the deformed configuration and $\mathbf{r} \wedge \mathbf{a}$ is a skew-symmetric tensor, such as $(\mathbf{r} \wedge \mathbf{a})\mathbf{w} = (\mathbf{r} \times \mathbf{a}) \times \mathbf{w}$, $\forall \mathbf{r}, \mathbf{a}, \mathbf{w} \in \mathcal{V}$.

Remark 2.1. The balance laws for linear and angular momenta lead to the existence of the Cauchy non-symmetric stress tensorial field, \mathbf{T} such that $\mathbf{T}\mathbf{n} = \mathbf{t}(\mathbf{n})$, and of the macro momentum, a third order tensor $\boldsymbol{\mu}$, which satisfies the relationship $\boldsymbol{\mu}\mathbf{n} = \mathbf{M}(\mathbf{n})$, and consequently *local balance equations for the linear and angular momentum* can be derived

$$\begin{aligned} \operatorname{div} \mathbf{T} + \hat{\rho} \mathbf{b} &= \hat{\rho} \mathbf{a}, \\ -2\mathbf{T}^a &= \operatorname{div} \boldsymbol{\mu} + \hat{\rho} \mathbf{B}_m. \end{aligned} \quad (2.6)$$

As a direct consequence of the balance equations written above, we write the balance equation

$$\operatorname{div} (\mathbf{T}^s - \frac{1}{2} \{\operatorname{div} \boldsymbol{\mu}\}^a) + \hat{\rho} \mathbf{b} = \hat{\rho} \mathbf{a}, \quad (2.7)$$

and the compatibility condition $\{\operatorname{div} \boldsymbol{\mu}\}^s + \hat{\rho} \mathbf{B}_m = 0$, if $\mathbf{B}_m \in \mathit{Sym}$ holds.

We describe the behaviour of an elasto-plastic material, as in Cleja-Țigoiu [8] and [9], based on the *existence of time dependent configurations with torsion*, denoted by $\mathcal{K}_t \equiv \mathcal{K}$. The configuration with torsion is viewed like a second order deformation, namely a pair of a second order tensor, called *plastic distortion* \mathbf{F}^p , and a third order tensor which is associated with the so-called *plastic connection with torsion* $\overset{(p)}{\boldsymbol{\Gamma}}$, in a local representation.

It is supposed that

- the material behaves like an hyperelastic (second order) material in terms of macroforces;

- lattice defects are modeled as differential geometry concepts;
- micro stress and stress momentum obey balance laws and satisfy the viscoplastic type constitutive equations, in \mathcal{K}_t ;
- energetic arguments, like the macro and micro balance equations and the energy imbalance principle are extended to incorporate the dissipated power during the irreversible behaviour cumulated by the developed defect mechanism as well as by the plastic mechanism.

The thermomechanical restrictions on the constitutive functions will be driven. Further more, the evolution equations for \mathcal{K}_t , namely for $(\mathbf{F}^p, \mathbf{\Gamma}^{(p)})$ as well as the evolution equations for defects will be derived in a form to be compatible with the reduced dissipation inequality.

The composition rule of second order gradients, has been reformulated for second order deformations in [7], [9], following Cross [12] and Wang [50]

$$(\mathbf{F}, \mathbf{\Gamma}) := (\mathbf{F}^e, \mathbf{\Gamma}_{\mathcal{K}}^{(e)}) \circ (\mathbf{F}^p, \mathbf{\Gamma}^{(p)}), \quad (2.8)$$

where

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^p, \quad \mathbf{F} = \nabla \chi, \quad (2.9)$$

with χ – motion of the body \mathcal{B} , the *multiplicative decomposition* for \mathbf{F} and

$$\mathbf{\Gamma} = \mathbf{F}^p \mathbf{\Gamma}_{\mathcal{K}}^{(e)} [(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}] + \mathbf{\Gamma}^{(p)}, \quad \mathbf{\Gamma} = \mathbf{F}^{-1} \nabla \mathbf{F}, \quad (2.10)$$

i.e. *the composition rule of the connections*.

The defects inside the microstructure of the elasto-plastic body will be defined in terms of the geometric characteristics of the local plastic connection. We assume that the *plastic connection is metric* with respect to the metric measure of the non-Riemannian dislocated space, namely to the plastically deformed configuration.

Definition 2.3. *The plastic connection $\mathbf{\Gamma}^{(p)}$ has metric property with respect to the plastic metric tensor $\mathbf{C}^p := (\mathbf{F}^p)^T \mathbf{F}^p$, if*

$$(\nabla \mathbf{C}^p) \mathbf{u} = (\mathbf{\Gamma}^{(p)} \mathbf{u})^T \mathbf{C}^p + \mathbf{C}^p (\mathbf{\Gamma}^{(p)} \mathbf{u}), \quad \forall \mathbf{u} \in \mathcal{V}. \quad (2.11)$$

Remark 2.2. If the plastic connection $\mathbf{\Gamma}^{(p)}$ has metric property then the covariant derivative of the metric tensor \mathbf{C}^p relative to the affine connection $\mathbf{\Gamma}^{(p)}$ is vanishing (like in the Riemannian geometry).

We introduce the Bilby's type connection, [4], by $\overset{(p)}{\mathcal{A}} := (\mathbf{F}^p)^{-1} \nabla \mathbf{F}^p$.

As a consequence of the hypotheses and definitions introduced above, we give the following theorem.

Theorem 2.3. *The plastic connection with metric property with respect to \mathbf{C}^p is represented under the form, see [8], [9]*

$$\overset{(p)}{\mathbf{\Gamma}} = \overset{(p)}{\mathcal{A}} + (\mathbf{C}^p)^{-1} (\mathbf{\Lambda} \times \mathbf{I}), \quad (2.12)$$

where the third order tensor $\mathbf{\Lambda} \times \mathbf{I}$ is defined by

$$((\mathbf{\Lambda} \times \mathbf{I})\mathbf{u})\mathbf{v} = \mathbf{\Lambda}\mathbf{u} \times \mathbf{v}, \quad \forall \mathbf{u}, \mathbf{v}. \quad (2.13)$$

$\mathbf{\Lambda} \in \text{Lin}$ is called the *disclination tensor*.

Lattice defects will be characterized in terms of the plastic connection and the Cartan torsion.

Definition 2.4. *The Cartan torsion \mathbf{S}^p , as a third order tensor, is given by*

$$(\mathbf{S}\mathbf{u})\mathbf{v} = (\overset{(p)}{\mathbf{\Gamma}} \mathbf{u})\mathbf{v} - (\overset{(p)}{\mathbf{\Gamma}} \mathbf{v})\mathbf{u}. \quad (2.14)$$

Theorem 2.4. *The second order torsion tensor \mathcal{N}^p , introduced by $\mathcal{N}^p(\mathbf{u} \times \mathbf{v}) = (\mathbf{S}^p\mathbf{u})\mathbf{v}$, is expressed by*

$$\mathcal{N}^p = (\mathbf{F}^p)^{-1} \text{curl}(\mathbf{F}^p) + (\mathbf{C}^p)^{-1} ((\text{tr } \mathbf{\Lambda})\mathbf{I} - (\mathbf{\Lambda})^T), \quad (2.15)$$

$$(\mathbf{S}^p\mathbf{u})\mathbf{v} = (\mathbf{F}^p)^{-1} (\text{curl}(\mathbf{F}^p) (\mathbf{u} \times \mathbf{v}) + (\mathbf{C}^p)^{-1} (\mathbf{\Lambda}\mathbf{u} \times \mathbf{v} - \mathbf{\Lambda}\mathbf{v} \times \mathbf{u})).$$

The following tensorial densities associated with the incompatible (defect) fields are introduced by

$$\boldsymbol{\alpha} := (\mathbf{F}^p)^{-1} \text{curl} \mathbf{F}^p, \quad \text{dislocation density,}$$

$$\boldsymbol{\alpha}^\Lambda := (\mathbf{C}^p)^{-1} (\text{tr } \mathbf{\Lambda} \mathbf{I} - (\mathbf{\Lambda})^T), \quad \text{disclination density.}$$

As a consequence, we define *Burgers and Frank vectors* in terms of the plastic distortion \mathbf{F}^p and plastic connection $\overset{(p)}{\mathbf{\Gamma}}$.

The Burgers vector is defined in terms of the plastic distortion \mathbf{F}^p and it is associated with a circuit C_0 in the reference configuration. Let \mathcal{A}_0 be a surface with normal \mathbf{N} , which is bounded by C_0 a closed curve in the reference configuration of the body. The Burgers vector associated with the circuit is defined by

$$\begin{aligned} \mathbf{b}_{\mathcal{K}} &\equiv \left\{ \int_{C_{\mathcal{K}}} d\mathbf{x}_{\mathcal{K}} \right\} = \int_{C_0} \mathbf{F}^p d\mathbf{X} = \int_{\mathcal{A}_0} (\text{curl}(\mathbf{F}^p)) \mathbf{N} dA = \\ &= \int_{\mathcal{A}_{\mathcal{K}}} \boldsymbol{\alpha}_{\mathcal{K}} \mathbf{n}_{\mathcal{K}} dA_{\mathcal{K}}. \end{aligned} \quad (2.16)$$

$\alpha_{\mathcal{K}}$ is called *dislocation density tensor*. Now we can introduce the expressions for the dislocation density tensor, namely:

- $\alpha_{\mathcal{K}} := \frac{1}{\det \mathbf{F}^p} (\text{curl}(\mathbf{F}^p))(\mathbf{F}^p)^T$, which is written in the configuration with torsion and is called *Noll's dislocation density*, and
- $\alpha := (\mathbf{F}^p)^{-1} \text{curl} \mathbf{F}^p$, written in the reference configuration.

Definition 2.5. *We say that \mathbf{F}^p characterizes a screw dislocation if the generated Burgers vector through a circuit with the appropriate normal \mathbf{N} is collinear with the normal, i.e. $\mathbf{b} \parallel \mathbf{N}$, and an edge dislocation if $\mathbf{b} \perp \mathbf{N}$.*

In order to introduce a definition for the Frank vector, we state the proposition

Proposition 2.1. *Let the curvature tensor that belongs to $\Lambda \times \mathbf{I}$ be calculated as in (2.3), and denoted by \mathcal{R}^Λ . Then there exists a second order tensor field \mathbf{r}^Λ such that the following relation hold*

$$\mathbf{r}^\Lambda(\mathbf{u} \times \mathbf{v}) = (\mathbf{C}^p \mathcal{R}^\Lambda \mathbf{u})\mathbf{v} \quad \text{and} \quad \mathbf{r}^\Lambda = \text{curl} \Lambda + (\text{Adj} \Lambda)^T. \quad (2.17)$$

Adjoint of Λ , denoted $\text{Adj}(\Lambda)$, is the second order tensor

$$(\Lambda \mathbf{u}, \Lambda \mathbf{v}, \mathbf{w}) := (\mathbf{u}, \mathbf{v}, (\text{Adj} \Lambda)\mathbf{w}), \quad \forall \quad \mathbf{u}, \mathbf{v}, \mathbf{w}. \quad (2.18)$$

The Frank vector is associated with a circuit C_0 in the reference configuration and is defined here by

$$\Omega_{\mathcal{K}} = \int_{C_0} \Lambda d\mathbf{X} = \int_{A_0} (\text{curl} \Lambda) \mathbf{N} dA = \int_{A_{\mathcal{K}}} \alpha_{\mathcal{K}}^\Lambda \mathbf{n}_{\mathcal{K}} dA_{\mathcal{K}}, \quad (2.19)$$

where the disclination density $\alpha_{\mathcal{K}}^\Lambda = \frac{1}{\det(\mathbf{F}^p)} (\text{curl} \Lambda)(\mathbf{F}^p)^T$ is defined in the configuration with torsion.

3. Incompatibilities in classical elasticity with small deformations

It is assumed that the displacement vector \mathbf{u} is twice continuously differentiable at any point of a simple connected body undergoing elasto-plastic deformation. The total distortion tensor $\mathbf{H} = \nabla \mathbf{u}$ is called *compatible*, since from (2.1) the compatibility condition for the distortion \mathbf{H} holds.

$$\text{curl} \mathbf{H} = 0 \quad (3.1)$$

In the elasto-plastic theory of dislocations, the plastic, \mathbf{H}^p , and the elastic \mathbf{H}^e , components of the displacement gradient \mathbf{H} do not satisfy the compatibility condition (3.1), they are *incompatible*,

$$\mathbf{H} = \mathbf{H}^e + \mathbf{H}^p, \quad \text{curl} \mathbf{H}^e = -\text{curl} \mathbf{H}^p = \alpha \neq 0. \quad (3.2)$$

Consequently the elastic and plastic distortions can not be derived from displacement vectors. Here $\boldsymbol{\alpha}$ is **Ney's dislocation density** and it provides the incompatibility of the elastic and plastic distortions. The continuity condition yields

$$\operatorname{div} \boldsymbol{\alpha} = 0. \quad (3.3)$$

Defining the strain tensor $\boldsymbol{\varepsilon}$ as the symmetric part of the distortion \mathbf{H} and the rotation tensor $\boldsymbol{\Omega}$ as its skew-symmetric part, the following equalities hold

$$\mathbf{H} = \boldsymbol{\varepsilon} + \boldsymbol{\Omega}, \quad \boldsymbol{\Omega} \mathbf{w} = \boldsymbol{\omega} \times \mathbf{w}, \quad \forall \mathbf{w} \in \mathcal{V}, \quad (3.4)$$

where $\boldsymbol{\omega}$ is coaxial vector with the skew-symmetric part $\boldsymbol{\Omega}$, and it is called the *rotation vector*.

Similar relationships with (3.2) can be derived for the elastic and plastic distortions, namely

$$\begin{aligned} \mathbf{H}^e &= \boldsymbol{\varepsilon}^e + \boldsymbol{\Omega}^e, & \boldsymbol{\varepsilon}^e &= \{\mathbf{H}^e\}^S, & \boldsymbol{\Omega}^e &= \{\mathbf{H}^e\}^a, \\ \mathbf{H}^p &= \boldsymbol{\varepsilon}^p + \boldsymbol{\Omega}^p, & \boldsymbol{\varepsilon}^p &= \{\mathbf{H}^p\}^S, & \boldsymbol{\Omega}^p &= \{\mathbf{H}^p\}^a, \end{aligned} \quad (3.5)$$

and the appropriate associated vectors

$$\boldsymbol{\Omega}^e \mathbf{w} = \boldsymbol{\omega}^e \times \mathbf{w}, \quad \boldsymbol{\Omega}^p \mathbf{w} = \boldsymbol{\omega}^p \times \mathbf{w}, \quad \forall \mathbf{w} \in \mathcal{V}. \quad (3.6)$$

Proposition 3.1. *The compatibility relationship (3.1) together with (3.4) becomes*

$$\operatorname{curl} \boldsymbol{\varepsilon} + \operatorname{div} \boldsymbol{\omega} \mathbf{I} - \nabla^T \boldsymbol{\omega} = 0. \quad (3.7)$$

Applying the *curl-trace procedure* to the elastic and plastic distortions we find the equations

$$\begin{aligned} \operatorname{curl} \boldsymbol{\varepsilon}^e + \operatorname{div} \boldsymbol{\omega}^e \mathbf{I} - \nabla^T \boldsymbol{\omega}^e &= \boldsymbol{\alpha}, & \operatorname{curl} \boldsymbol{\varepsilon}^p + \operatorname{div} \boldsymbol{\omega}^p \mathbf{I} - \nabla^T \boldsymbol{\omega}^p &= -\boldsymbol{\alpha}, \\ \operatorname{div} \boldsymbol{\omega}^e &= -\operatorname{div} \boldsymbol{\omega}^p = \frac{1}{2} \operatorname{tr} \boldsymbol{\alpha}. \end{aligned} \quad (3.8)$$

The equivalent relationships to (3.8) can be derived under the form

$$\nabla \boldsymbol{\omega}^e = (\operatorname{curl} \boldsymbol{\varepsilon}^e)^T + \mathbf{K}, \quad \nabla \boldsymbol{\omega}^p = (\operatorname{curl} \boldsymbol{\varepsilon}^p)^T - \mathbf{K}, \quad \mathbf{K} = \frac{1}{2} \operatorname{tr} \boldsymbol{\alpha} \mathbf{I} - \boldsymbol{\alpha}^T, \quad (3.9)$$

in terms of \mathbf{K} , which is called *Ney curvature tensor*.

With the definition of the elastic, κ^e , and plastic, κ^p , curvature tensors by

$$\kappa^e = \nabla \boldsymbol{\omega}^e, \quad \kappa^p = \nabla \boldsymbol{\omega}^p, \quad (3.10)$$

if we take the *curl* of the relationships (3.6) together with (3.8) we find

$$\begin{aligned}\operatorname{curl}\boldsymbol{\kappa}^e &= \operatorname{curl}(\operatorname{curl}\boldsymbol{\varepsilon}^e)^T + \operatorname{curl}\mathbf{K} = 0 \\ \operatorname{curl}\boldsymbol{\kappa}^p &= \operatorname{curl}(\operatorname{curl}\boldsymbol{\varepsilon}^p)^T - \operatorname{curl}\mathbf{K} = 0.\end{aligned}\tag{3.11}$$

Remark 3.1. Thus, in the small elasto-plastic framework of dislocations the elastic and plastic curvatures $(\boldsymbol{\kappa}^e, \boldsymbol{\kappa}^p)$ are *curl-free*, but the plastic and elastic distortions are incompatible. de Wit in [13] introduced the *hypothesis: the elastic and plastic curvatures $(\boldsymbol{\kappa}^e, \boldsymbol{\kappa}^p)$ are not curl-free*. Consequently the possibility of a rotational incompatibility is certificated, i.e. a non-zero tensor $\boldsymbol{\theta} \neq 0$ exists such that

$$\boldsymbol{\theta} = \operatorname{curl}\boldsymbol{\kappa}^e = -\operatorname{curl}\boldsymbol{\kappa}^p.\tag{3.12}$$

Substituting the elastic and plastic curvature, (3.10), in the equation (3.8) the modified equations are derived

$$\operatorname{curl}\boldsymbol{\varepsilon}^e = \boldsymbol{\alpha} + (\boldsymbol{\kappa}^e)^T - \operatorname{tr}(\boldsymbol{\kappa}^e)\mathbf{I}, \quad \operatorname{curl}\boldsymbol{\varepsilon}^p = -\boldsymbol{\alpha} + (\boldsymbol{\kappa}^p)^T - \operatorname{tr}(\boldsymbol{\kappa}^p)\mathbf{I},\tag{3.13}$$

These formulae are attributed in the literature to Arsenlis and Parks [3], but they go back to de Wit [13]. The equations (3.13) defines the incompatibility of the plastic strain $\boldsymbol{\eta}$, in terms of the dislocation density tensor $\boldsymbol{\alpha}$ and the curvature tensor \mathbf{K} . The incompatibility tensor $\boldsymbol{\eta}$ is defined as

$$\boldsymbol{\eta} = \operatorname{curl}(\operatorname{curl}\boldsymbol{\varepsilon}^p)^T, \quad \text{and} \quad \boldsymbol{\eta} = \operatorname{curl}\mathbf{K} - \boldsymbol{\theta}.\tag{3.14}$$

Remark 3.2. *If the elastic distortion is compatible, then $\boldsymbol{\alpha} = \operatorname{curl}\mathbf{H}^e = 0$ and the elastic strain is compatible if and only if $\operatorname{curl}(\operatorname{curl}\boldsymbol{\varepsilon}^e)^T = 0$. We can prove*

Proposition 3.2. *The following formula*

$$\operatorname{curl}\mathbf{H}^p = \operatorname{curl}\boldsymbol{\varepsilon}^p + \operatorname{tr}(\nabla\boldsymbol{\omega}^p)\mathbf{I} - (\nabla\boldsymbol{\omega}^p)^T,\tag{3.15}$$

$$\text{or} \quad \operatorname{curl}\{\mathbf{H}^p\}^a = \operatorname{tr}(\nabla\boldsymbol{\omega}^p)\mathbf{I} - (\nabla\boldsymbol{\omega}^p)^T,$$

is valid and expresses the $\operatorname{curl}\mathbf{H}^p$ in terms of $\operatorname{curl}\boldsymbol{\varepsilon}^p$ and $\nabla\boldsymbol{\omega}^p$.

de Wit (1970) in [13], see also [24], reviewed the compatibility conditions for the distortion \mathbf{H} , the strain $\boldsymbol{\varepsilon}$, the rotation $\boldsymbol{\omega}$, and the bent-twist $\boldsymbol{\kappa}$, within the classical elasticity, with small deformation, and formulated the proposition, written below.

Proposition 3.3. *Suppose that the smooth fields $\boldsymbol{\kappa}$ and $\boldsymbol{\alpha}$ are known and satisfy in a simply-connected domain, say \mathcal{V} , the conditions*

$$\operatorname{curl}\boldsymbol{\kappa} = 0, \quad \boldsymbol{\alpha} = 0.\tag{3.16}$$

Then there exists the rotation vector $\boldsymbol{\omega}$ and the displacement vector \mathbf{u} , for the compatible deformation, defined on a simple-connected domain. In order to find their spatial dependence it is only necessary to know $\boldsymbol{\omega}$ and \mathbf{u} at some particular point \mathbf{x}_0 .

The statements are direct consequences of the formulae written above, using also (3.13). For every closed curve $\mathcal{C} \subset \mathcal{V}$, and a surface $\mathcal{S} \subset \mathcal{V}$, which is bounded by \mathcal{C} , it follows

$$\begin{aligned} \mathbf{u}(\mathbf{x}) &= \mathbf{u}(\mathbf{x}_0) + \int_{\mathcal{C}} \boldsymbol{\epsilon} \, d\mathbf{y} + \int_{\mathcal{C}} \boldsymbol{\omega} \times d\mathbf{y} = \\ &= \mathbf{u}(\mathbf{x}_0) + \boldsymbol{\omega}_0 \times (\mathbf{x} - \mathbf{x}_0) + \int_{\mathcal{S}} \text{curl} \boldsymbol{\epsilon} \, \mathbf{n} \, dA \\ &\quad + \int_{\mathcal{S}} (\mathbf{y} - \mathbf{x}) \times (\text{curl} \boldsymbol{\kappa} \, \mathbf{n}) \, dA + \int_{\mathcal{S}} ((\text{tr} \boldsymbol{\kappa}) \mathbf{I} - \boldsymbol{\kappa}^T) \, \mathbf{n} \, dA, \end{aligned} \quad (3.17)$$

$$\boldsymbol{\omega}(\mathbf{x}) = \boldsymbol{\omega}(\mathbf{x}_0) + \int_{\mathcal{C}} \boldsymbol{\kappa} \, d\mathbf{x} = \boldsymbol{\omega}(\mathbf{x}_0) + \int_{\mathcal{S}} \text{curl} \boldsymbol{\kappa} \, \mathbf{n} \, dA, \quad (3.18)$$

by applying Stokes formulae for any surface \mathcal{S} bounded by the curve \mathcal{C} , and which is inside the domain. Here \mathbf{n} is the unit normal vector at the surface, \mathbf{x}_0 is a fixed point on an arbitrary curve \mathcal{C} (not necessarily closed) and \mathbf{x} is a current point on \mathcal{C} .

Burgers vector and Frank vector are given by integral along a closed curve, called circuit, \mathcal{C}

$$\mathbf{b} = \int_{\mathcal{C}} (\boldsymbol{\epsilon} + \mathbf{x} \times \boldsymbol{\omega}) \, d\mathbf{y}, \quad \boldsymbol{\Omega} = \int_{\mathcal{C}} \boldsymbol{\kappa} \, d\mathbf{x}, \quad (3.19)$$

By applying the Stokes formulae for any surface \mathcal{S} bounded by the curve \mathcal{C} , and which is inside the domain, it follows that

$$\begin{aligned} \mathbf{b} &= \int_{\mathcal{S}} (\boldsymbol{\alpha} + \mathbf{x} \times \text{curl} \boldsymbol{\kappa}) \, \mathbf{n} \, dA, \\ \boldsymbol{\Omega} &= \int_{\mathcal{S}} \text{curl} \boldsymbol{\kappa} \, \mathbf{n} \, dA, \end{aligned} \quad (3.20)$$

where $\boldsymbol{\alpha} = \text{curl} \boldsymbol{\epsilon} + (\text{tr} \boldsymbol{\kappa}) \mathbf{I} - (\boldsymbol{\kappa})^T$. Here the following **interpretation** can be given: $\boldsymbol{\Omega}$ is the vector associated with the disclination crossing the surface \mathcal{S} , while \mathbf{b} is the general Burgers vector associated with the dislocation and disclination crossing the surface \mathcal{S} .

Remark 3.3. If \mathcal{C} is *irreducible*, i.e. the curve can not be deformed continuously into a point without leaving the definition domain, \mathbf{u} and $\boldsymbol{\omega}$ may not

return to their original values following the circuit. The changing are given as a consequence of (3.17) and (3.18), when \mathbf{x} is taken to be \mathbf{x}_0 ,

$$[\mathbf{u}] = \int_{\mathcal{C}} \boldsymbol{\epsilon} d\mathbf{y} + \int_{\mathcal{C}} (\mathbf{y} - \mathbf{x}_0) \times \boldsymbol{\kappa} d\mathbf{y}, \quad [\boldsymbol{\omega}] = \int_{\mathcal{C}} \boldsymbol{\kappa} d\mathbf{x} \quad (3.21)$$

The expression has been rewritten by de Wit [13] as follows

$$[\mathbf{u}] = \mathbf{b} + \mathbf{x}_0 \times \boldsymbol{\Omega}, \quad [\boldsymbol{\omega}] = [\boldsymbol{\Omega}] \quad \text{were} \quad (3.22)$$

$$\boldsymbol{\Omega} = \int_{\mathcal{C}} \boldsymbol{\kappa} d\mathbf{x}, \quad \mathbf{b} = \int_{\mathcal{C}} \boldsymbol{\epsilon} d\mathbf{y} + \int_{\mathcal{C}} \mathbf{y} \times \boldsymbol{\kappa} d\mathbf{y}$$

Moreover, \mathbf{b} and $\boldsymbol{\Omega}$ remain unchanged if \mathcal{C} is deformed continuously into an other one, without leaving the domain.

Finally let us consider the volume \mathcal{V} bounded by the surface \mathcal{S} . By applying the divergence theorem the following conditions hold

$$\mathbf{b} = \int_{\mathcal{V}} (\text{div} \boldsymbol{\alpha} + \mathbf{x} \times \text{div} \boldsymbol{\theta} + 2 \langle \boldsymbol{\theta} \rangle) dV, \quad (3.23)$$

$$\boldsymbol{\Omega} = \int_{\mathcal{V}} \text{div} \boldsymbol{\theta} dV, \quad \boldsymbol{\theta} = \text{curl} \boldsymbol{\kappa},$$

where $\langle \boldsymbol{\theta} \rangle$ is the coaxial vector associated with the skew-symmetric tensor $\{\boldsymbol{\theta}\}^a$, namely $(\{\boldsymbol{\theta}\}^a) \mathbf{w} = \langle \boldsymbol{\theta} \rangle \times \mathbf{w}, \quad \forall \mathbf{w}$.

4. Small elastic and plastic distortions derived from the finite kinematics

In the case of small elastic and plastic distortion we adopt the basic hypotheses

$$\mathbf{F} = \mathbf{I} + \nabla \mathbf{u}, \quad \|\nabla \mathbf{u}\| \ll 1, \quad (4.1)$$

$$\mathbf{F}^e = \mathbf{I} + \mathbf{H}^e, \quad \mathbf{F}^p = \mathbf{I} + \mathbf{H}^p, \quad \|\mathbf{H}^e\| \ll 1, \quad \|\mathbf{H}^p\| \ll 1,$$

lead to

$$\mathbf{H} = \mathbf{H}^e + \mathbf{H}^p, \quad \text{with} \quad \mathbf{H} = \nabla \mathbf{u} \quad (4.2)$$

$$\text{curl} \mathbf{H}^e = -\text{curl} \mathbf{H}^p \neq 0.$$

Under the hypothesis of small distortions, the consequences that follow from the constitutive framework of finite deformations can be summarized as follows:

- the connections are expressed by

$$\mathbf{\Gamma} = \nabla \mathbf{H}, \quad \overset{(p)}{\mathbf{\Gamma}} = \nabla \mathbf{H}^p + \mathbf{\Lambda} \times \mathbf{I}, \quad \overset{(e)}{\mathbf{\Gamma}} = \nabla \mathbf{H}^e - \mathbf{\Lambda} \times \mathbf{I}, \quad (4.3)$$

$\nabla \mathbf{H}^p, \nabla \mathbf{H}^e, \mathbf{\Lambda}$ having the same order of magnitude;

- Bilby's connection and plastic Cauchy- Green tensor become

$$\overset{(p)}{\mathbf{A}} := \nabla \mathbf{H}^p, \quad \mathbf{C}^p = \mathbf{I} + 2\boldsymbol{\varepsilon}^p, \quad \boldsymbol{\varepsilon}^p = \frac{1}{2}(\nabla \mathbf{H}^e + (\nabla \mathbf{H}^e)^T). \quad (4.4)$$

- the second order torsion \mathcal{N}^p which is associated with Cartan torsion \mathbf{S}^p by $(\mathbf{S}^p \mathbf{u}) \mathbf{v} = \mathcal{N}^p(\mathbf{u} \times \mathbf{v})$, is expressed by

$$\begin{aligned} \mathcal{N}^p &= \text{curl} \mathbf{H}^p + ((\text{tr } \mathbf{\Lambda}) \mathbf{I} - \mathbf{\Lambda}^T), \quad \text{and similarly} \\ \mathcal{N}^e &= \text{curl} \mathbf{H}^e - ((\text{tr } \mathbf{\Lambda}) \mathbf{I} - \mathbf{\Lambda}^T). \end{aligned} \quad (4.5)$$

Using the decomposition of plastic part of the deformation gradient into its symmetric and skew-symmetric parts and applying the *curl-trace procedure* (3.8) we can prove the following result

Theorem 4.1. *There exists $\boldsymbol{\kappa}^p$ such that the second order torsion \mathcal{N}^p is given by*

$$\mathcal{N}^p = \text{curl} \boldsymbol{\varepsilon}^p + (\text{tr } \boldsymbol{\kappa}^p) \mathbf{I} - (\boldsymbol{\kappa}^p)^T, \quad \text{where } \boldsymbol{\kappa}^p = \underbrace{\mathbf{\Lambda}} + \underbrace{\nabla \boldsymbol{\omega}^p}, \quad (4.6)$$

$$\text{or equivalently } \boldsymbol{\kappa}^p = (\text{curl} \boldsymbol{\varepsilon}^p)^T + \mathcal{N}^p - \frac{1}{2} (\text{tr } \mathcal{N}^p) \mathbf{I}.$$

Remark 4.1. We derived that $\boldsymbol{\kappa}^p$ contains

$\underbrace{\mathbf{\Lambda}}$ – an incompatible part and $\underbrace{\nabla \boldsymbol{\omega}^p}$ – a compatible part.

Thus $\boldsymbol{\kappa}$ is not a *curl-free* tensor, since $\boldsymbol{\theta} = \text{curl} \boldsymbol{\kappa} = \text{curl} \mathbf{\Lambda}$, where

$$\boldsymbol{\theta}(\mathbf{u} \times \mathbf{v}) \cdot (\mathbf{w} \times \mathbf{z}) = ((\mathcal{R} \mathbf{u}) \mathbf{v}) \mathbf{w} \cdot \mathbf{z}. \quad (4.7)$$

Consequently, under the hypothesis of small elasto-plastic distortions the formulae which characterize the framework of second order finite elasto-plasticity allow us to prove the existence of a second order tensor, which leads to a non-vanishing *curl*, i.e. $\text{curl} \mathbf{\Lambda} \neq 0$. A similar result follows for the elastic part.

Proposition 4.1. *There exists a second order tensor $\boldsymbol{\kappa}^e$ such that the following relationship holds*

$$\mathcal{N}^e = \text{curl} \boldsymbol{\varepsilon}^e - (\text{tr } \boldsymbol{\kappa}^e) \mathbf{I} - (\boldsymbol{\kappa}^e)^T, \quad \text{where } \boldsymbol{\kappa}^e = -\mathbf{\Lambda} + \nabla \boldsymbol{\omega}^e. \quad (4.8)$$

Remark 4.2. As a direct consequence of the formulae (4.5), which characterize the second order torsion tensor in terms of the elastic and plastic small distortions and the disclination tensor, it result

$$\mathcal{N}^p + \mathcal{N}^e = 0, \quad \boldsymbol{\kappa}^e + \boldsymbol{\kappa}^p = \nabla \boldsymbol{\omega}. \quad (4.9)$$

Remark 4.3. Let us suppose that the plastic connection satisfies the compatibility condition (2.2), having the non-zero torsion. In the paper by Cleja-Țigoiu et al [11] it is provided an equivalent representation for a such plastic connection.

The connection $\boldsymbol{\Gamma}$ with torsion, that can be expressed by

$$\mathbf{U}^p \overset{(p)}{\boldsymbol{\Gamma}} = \widehat{\boldsymbol{\Lambda}} \times \mathbf{U}^p + ((\nabla \mathbf{U}^p), \quad (\mathbf{U}^p)^2 = \mathbf{C}^p, \quad \widehat{\boldsymbol{\Lambda}} \in Lin, \quad (4.10)$$

satisfies the integrability condition (2.2) if and only if $\widehat{\boldsymbol{\Lambda}}$ is a solution of the equation (2.17)₁ for $\mathbf{r}^\Lambda = 0$, while the *second order torsion* \mathbf{N}^p and $\widehat{\boldsymbol{\Lambda}}$ are related by the relationship

$$\mathbf{C}^p \mathbf{N}^p = \det \mathbf{U}^p \{ \text{tr}(\widehat{\boldsymbol{\Lambda}}(\mathbf{U}^p)^{-1}) \mathbf{I} - ((\mathbf{U}^p)^{-1} \widehat{\boldsymbol{\Lambda}})^T \} + \mathbf{U}^p (\text{curl} \mathbf{U}^p), \quad (4.11)$$

Let us remark here that in the case of small elastic and plastic distortions if we compare (4.10) with (2.12), we derive from (4.11) the expression (4.6) for the second order torsion tensor. Now $\boldsymbol{\kappa}^p$ is identified with $\widehat{\boldsymbol{\Lambda}}$. As a conclusion (4.10) becomes $\overset{(p)}{\boldsymbol{\Gamma}} = \nabla \boldsymbol{\varepsilon}^p + \widehat{\boldsymbol{\Lambda}} \times \mathbf{I}$, and $\widehat{\boldsymbol{\Lambda}} = \boldsymbol{\Lambda} + \nabla \boldsymbol{\omega}^p$, with $\boldsymbol{\Lambda}$ the disclination tensor which enters (4.3)₂.

5. Modeling structural defects. Different approaches

5.1. Elastic Models of Crystal Defects

• **de Wit point of view.** The compatibility conditions for the basic fields written in (3.1) are violated for incompatible elastic materials or for the elastic materials with defects. The disclinations are defined by de Wit in a similar way like the dislocations, see de Wit [13], [14].

For an elastic material with discrete defects, like straight dislocations or straight disclinations, the defect region is cut of the body and the elastic body is reduced to a multiply-connected domain, where the compatibility conditions are satisfied. To solve the problem, the body is cut along a certain surface in such a way that body becomes simply-connected. However on the two-sided surface the jump conditions are written under the form (3.22) in terms of the constants, $\mathbf{b}, \boldsymbol{\Omega}$, that is Burgers vector and Frank vector given by integral along an appropriate circuit, \mathcal{C} .

In a series of papers [13] - [16] de Wit debated different aspects related to the theory of disclinations, within small deformation elasto-plastic formalism, and developed models for discrete (straight lines and loops) and

continuous disclinations, in terms of defect densities. When the disclination densities are vanishing the theory of dislocations is derived as a peculiar case. Moreover, it is proved in [14] that always it is possible to associate for every disclination line a *dislocation model, which is a wall terminating on the line*. de Wit in [15] developed the theory of structural defects for a linear elastic, infinitely extended, homogeneous and isotropic body. The integral expressions are derived for the total displacement, elastic strain $\boldsymbol{\varepsilon}^e$, the bent-twist (curvature) $\boldsymbol{\kappa}$ and the stress.

The plastic problem is solved: for a given plastic strain $\boldsymbol{\varepsilon}^p$ as a function of the space, find the resulting total displacement field \mathbf{u} . The Green function for the isotropic linear elastic material is essentially used in order to find the solution.

The incompatibility problem is solved: for a given incompatibility tensor $\boldsymbol{\eta} = \text{curl}(\text{curl}\boldsymbol{\varepsilon}_p)^T$ - see (3.14), as a function of the space, find the resulting elastic strain $\boldsymbol{\varepsilon}^e$. The mentioned results are reduced to those for the dislocation theory when the disclinations vanish. In [15] the problems have been solved without any specification of the nature of the defect involved.

As a principal result: if the basic plastic fields $\boldsymbol{\varepsilon}^p, \boldsymbol{\kappa}^p$ or the defect densities $\boldsymbol{\alpha}, \boldsymbol{\theta}$ are given as prescribed function of space, find the elastic field $\boldsymbol{\varepsilon}^e, \boldsymbol{\kappa}^e$.

- **Teodosiu point of view.** The elastic model of crystal defects are elaborated by Teodosiu in [44], when $\kappa = 0$, i.e. only dislocations are taken into account.

- **Mura point of view:** Burgers vector and Frank vector are given by integral lines along the circuit \mathcal{C} , in an incompatible simply-connected domain. The *plastic distortion* and *plastic rotation* were defined by Mura [35], as *distribution* with support on the surface S , denoted by $\delta(S)$, containing the defects,

$$\begin{aligned}\boldsymbol{\beta}^*(\mathbf{x}) &\equiv -\delta(S)\mathbf{n} \otimes \{\mathbf{b} + (\mathbf{x} - \mathbf{x}_0) \times \boldsymbol{\Omega}\}, \\ \boldsymbol{\Phi}^*(\mathbf{x}) &\equiv \delta(S)\mathbf{n} \otimes \boldsymbol{\Omega}.\end{aligned}\tag{5.1}$$

These quantities have been interpreted by de Wit, see [14], [16] as the *dislocation and disclination loop densities*

$$\boldsymbol{\varepsilon}^p = \boldsymbol{\beta}^*, \quad \boldsymbol{\kappa}^p = \text{curl}\boldsymbol{\beta}^* + \boldsymbol{\Phi}^*.\tag{5.2}$$

In Mura [36] a line defect containing both dislocations and disclinations is described in analytical derivation, by solving appropriate elastic boundary values problems, with the plastic incompatibilities viewed as sources. In the other words, Mura investigated the methods of finding the associated elastic fields (displacements, strains, stresses) and related problems for given distributions of $\boldsymbol{\varepsilon}^*$, called *eigenstrain*. Particular attention is payed to the

case when an uniform $\boldsymbol{\varepsilon}^*$ is placed in an ellipsoidal domain in an infinitely extended medium, i.e. the *ellipsoidal inclusion problem*.

The elastic type constitutive equation relates the elastic strain to the stress $\boldsymbol{\sigma}$, say by an anisotropic linear elastic law

$$\boldsymbol{\sigma} = \mathcal{C}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p), \quad \text{since} \quad \boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p. \quad (5.3)$$

The equilibrium equation together with (5.3) is

$$\operatorname{div} \boldsymbol{\sigma} = 0 \quad \iff \quad \operatorname{div} \mathcal{C}(\boldsymbol{\varepsilon}) = \operatorname{div} \mathcal{C}(\boldsymbol{\varepsilon}^p), \quad (5.4)$$

in which $\boldsymbol{\varepsilon}$ is replaced by the gradient of the displacement vector, \mathbf{u} . Mura solves the following problem

Problem: Given the plastic strain $\boldsymbol{\varepsilon}^p, \boldsymbol{\kappa}^p$ find the displacement field $\mathbf{u} : \mathcal{B} \times R \rightarrow \mathcal{V}$ such that the equilibrium equation be satisfied

$$\operatorname{div} \mathcal{C}\{\nabla \mathbf{u}\} = \operatorname{div} \mathcal{C}(\boldsymbol{\varepsilon}^p) \quad (5.5)$$

as well as the appropriate boundary conditions (say stress free)

$$\mathcal{C}(\boldsymbol{\varepsilon})\mathbf{n} = \mathcal{C}(\boldsymbol{\varepsilon}^p)\mathbf{n}. \quad (5.6)$$

5.2. Small deformations elasto-plastic models

5.2.1. Mayeur, McDowell and Bammann' model for dislocations

We present some aspects related to the models proposed in the papers by Mayeur et al. [29], [30], namely a slip gradient-based extended crystal plasticity, within the small deformation framework. The model is used to simulate the mechanical response of a single crystal with a single active slip system, and two types of dislocation measures. Concerning the micro boundary conditions two types of null-working conditions are considered for modeling the interfaces

- the *microhard* condition, that is intended to represent the case where dislocations are *unobstructed at the interface* (free surface)
- *microfree* condition, which is intended to represent the case where dislocations are *blocked*.

In addition to the formulae concerning the incompatibility in classical elasticity, (3.1)-(3.6), (3.11), some hypotheses are introduced under the form of axioms.

Ax. 1 A continuum measure of the deformation incompatibility is the geometrical necessary dislocation (GND) density tensor $\boldsymbol{\alpha}$, introduced in (3.10)

$$\boldsymbol{\alpha} = -\operatorname{curl} \mathbf{H}^e = \operatorname{curl} \mathbf{H}^p. \quad (5.7)$$

Ax. 2 The so-called GND density tensor is written in the form which appears in Arsenlis and Parks [3]

$$\boldsymbol{\alpha} = b \sum_{\alpha} (\rho_{G,\perp}^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{t}^{\alpha} + \rho_{G,\odot}^{\alpha} \mathbf{s}^{\alpha} \otimes \mathbf{s}^{\alpha}), \quad (5.8)$$

where $\mathbf{t}^{\alpha} = \mathbf{s}^{\alpha} \times \mathbf{n}^{\alpha}$, b is the magnitude of Burgers vector, and the edge, $\rho_{G,\perp}^{\alpha}$, and screw, $\rho_{G,\odot}^{\alpha}$, GND densities are defined *as gradients of slip projected in the glide directions for pure edge and screw dislocations*, i.e.

$$\rho_{G,\perp}^{\alpha} = -\frac{1}{b} \nabla \gamma^{\alpha} \cdot \mathbf{s}^{\alpha}, \quad \rho_{G,\odot}^{\alpha} = \frac{1}{b} \nabla \gamma^{\alpha} \cdot \mathbf{t}^{\alpha}, \quad (5.9)$$

where γ^{α} are plastic shears. The relation incorporate non-local effect into the slip system hardening description, through the gradient of the plastic shear. A similar formula is given in Kuroda and Tveergard ([28]), where the rate or the GND densities are described directly in terms of the gradient of plastic shear rates.

Ax. 3 The balance equation for Cauchy stress $div \mathbf{T} + \mathbf{b} = \mathbf{0}$, \mathbf{T} symmetric.

Ax. 4 The dissipation inequality, which states that the deformation power $\mathbf{T} \cdot \dot{\boldsymbol{\varepsilon}}$ must be greater than or equal to the rate of change in the free energy of the system, $\dot{\psi}$, namely $\mathbf{T} \cdot \dot{\boldsymbol{\varepsilon}} - \dot{\psi} \geq 0$. In the model the free energy density $\psi = \psi(\boldsymbol{\varepsilon}^e, \zeta^{\alpha})$, is a function of elastic strain as well as of the scalar strain-like internal state variables $\zeta_l^{\alpha}, l..$, with the particular case

$$\psi = \frac{1}{2} \boldsymbol{\varepsilon}^e \cdot \mathcal{C} \boldsymbol{\varepsilon}^e + \frac{1}{2} \mu \sum_{\alpha} (\zeta^{\alpha})^2. \quad (5.10)$$

Then the constitutive restriction are given by

$$\mathbf{T} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}^e}, \quad \xi_l^{\alpha} = \rho \frac{\partial \psi}{\partial \zeta_l^{\alpha}}, \quad (5.11)$$

ξ_l^{α} are the thermodynamic forces work-conjugate to the thermodynamic displacements, ζ_l^{α} .

Ax. 5 The evolution equations for the plastic strain

$$\dot{\boldsymbol{\varepsilon}}^p = \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{N}^{\alpha}, \quad \mathbf{N}^{\alpha} = \{\mathbf{s}^{\alpha} \otimes \mathbf{n}^{\alpha}\}^S, \quad (5.12)$$

where the yield function F^{α} with the resolved shear stress τ^{α} are defined by $F^{\alpha} = |\tau^{\alpha} - \tau_b| - r^{\alpha}$, $\tau^{\alpha} = \mathbf{s}^{\alpha} \cdot \mathbf{T} \mathbf{n}^{\alpha}$, and for

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{F^{\alpha}}{g^{\alpha}} \right)^m. \quad (5.13)$$

In these equation g^{α} is the drag stress, τ_b is the back stress, r^{α} is the threshold stress which is given by the Taylor relation

$$r^{\alpha} = \mu c_1 b \sqrt{\sum_{\beta} h^{\alpha\beta} \rho^{\beta}}, \quad \zeta^{\alpha} = c_1 b \sqrt{\sum_{\beta} h^{\beta} \rho^{\beta}}, \quad (5.14)$$

c_1 is a material constant related to the dislocation configuration, ρ^β is the total dislocation density on the slip system β .

The microstructural evolution is related to the change in the dislocated state of the crystal, and the total dislocation density on each system is assumed to be additively decomposed into *statistically stored dislocation* (SSD) and GND densities, namely $\rho^\alpha = \rho_S^\alpha + \rho_G^\alpha$. The SSD evolves as it is described by Kocks and Mecking in [34]

$$\dot{\rho}_S^\alpha = (c_2 \sqrt{\sum_{\beta} a^{\alpha\beta} \rho^\beta} - c_3 \rho_S^\alpha) |\dot{\gamma}^\alpha|. \quad (5.15)$$

The total GND density on the slip system is taken to be given as in Arsenlis and Parks [3]

$$\rho_G^\alpha = \sqrt{(\rho_{G,\perp}^\alpha)^2 + (\rho_{G,\odot}^\alpha)^2}, \quad (5.16)$$

together with (5.9).

We remark that it would be necessary to study the compatibility between the evolution equations for the dislocation densities, namely the rates of stored energy due to local (SSD) (69) and nonlocal (GND) micro structure evolution generated by (70), respectively, and the postulated form for the evolution of the plastic strain (5.12).

5.2.2. Model proposed by Fressengeas, Taupin, Capolungo [19]

In [19], Fressengeas et al. proposed a complex model accounting for the dislocations and disclinations, that is for structural defects, in the case of small deformations. The aim of the paper was to present both the translational and rotational aspects of lattice incompatibilities. The non-symmetric Cauchy stress and couple stresses have been considered in the problem.

The following notation has been introduced in the paper - the cross product of a second order tensor \mathbf{A} and a vector \mathbf{u} is a tensor, denoted by $\mathbf{A} \times \mathbf{u}$, and defined by: $(\mathbf{A} \times \mathbf{u})^T \mathbf{w} = (\mathbf{A}^T \mathbf{u}) \times \mathbf{w}$, for all vectors \mathbf{w} .

They supposed that the non-symmetric Cauchy stress tensor, \mathbf{T} , and the couple stress tensor \mathbf{m} (i.e. a second order field) satisfy macro balance equations given in Fleck et al. [18]

$$\operatorname{div} \mathbf{T} = 0, \quad \operatorname{div} \mathbf{m} + 2 \langle \mathbf{T}^a \rangle = 0, \quad (5.17)$$

where $\langle \mathbf{T}^a \rangle$ is the coaxial vector associated with the skew-symmetric part of \mathbf{T} . The constitutive relationships are considered to be written under the form

$$\begin{aligned} \mathbf{T} &= \mathcal{E}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) + \mathcal{D}(\nabla \boldsymbol{\omega} - \boldsymbol{\kappa}^p), \\ \mathbf{m} &= \mathcal{A}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) + \mathcal{B}(\nabla \boldsymbol{\omega} - \boldsymbol{\kappa}^p), \end{aligned} \quad (5.18)$$

where $\{\nabla \mathbf{u}\}^a \mathbf{v} = \boldsymbol{\omega} \times \mathbf{v}, \forall \mathbf{v}$. The system to define the principal fields $\boldsymbol{\varepsilon}^p, \boldsymbol{\kappa}^p$, and the incompatibilities $\boldsymbol{\alpha}, \boldsymbol{\theta}$, is given by

$$\begin{aligned} \boldsymbol{\alpha} &= -\text{curl} \boldsymbol{\varepsilon}^p + \boldsymbol{\kappa}^{pT} - \text{tr}(\boldsymbol{\kappa}^p) \mathbf{I}, \quad \boldsymbol{\theta} = -\text{curl}(\boldsymbol{\kappa}^p), \\ \dot{\boldsymbol{\kappa}}^p &= \boldsymbol{\theta} \times \frac{1}{B_\theta} \langle \mathbf{m}^T \boldsymbol{\theta} \rangle, \\ \dot{\boldsymbol{\varepsilon}}^p &= \frac{1}{2} (\boldsymbol{\alpha} \times \frac{1}{B_\alpha} \langle \{\mathbf{T}\}^a \boldsymbol{\alpha} \rangle + (\boldsymbol{\alpha} \times \frac{1}{B_\alpha} \langle \{\mathbf{T}\}^a \boldsymbol{\alpha} \rangle)^T). \end{aligned} \quad (5.19)$$

We denoted by $\langle \mathbf{m}^T \boldsymbol{\theta} \rangle$ and $\langle \{\mathbf{T}\}^a \boldsymbol{\alpha} \rangle$ the coaxial vectors associated with the skew-symmetric part of the written tensors into the brackets. B_α and B_θ are positive material parameters.

In order to formulate the initial and boundary value problem, the macroscopic boundary conditions have to be introduced in terms of the given values for the vector stress and couple stress vector, or for the given displacement. The initial values for the basic fields $\boldsymbol{\varepsilon}^p, \boldsymbol{\kappa}^p$ are necessary in connection with the evolution equations, (5.19), which are introduced in the model.

As peculiar aspects related to the proposed models we remark that,

- the free energy density has been proposed as a function of elastic strain and elastic curvature, $\psi = \psi(\boldsymbol{\varepsilon}^e, \boldsymbol{\kappa}^e)$;

- the derived constitutive relationships (5.18) are linearly with respect to elastic strain, $\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p$, and elastic curvature tensor, $\boldsymbol{\kappa}^e = \nabla \boldsymbol{\omega} - \boldsymbol{\kappa}^p$, if the free energy density is anisotropic and quadratic in their arguments. The constitutive equations involve the characteristic lengths and have non-local character;

- the incompatibility tensors are considered to be the dislocation and disclination densities, $\boldsymbol{\alpha}, \boldsymbol{\theta}$, and are described by appropriate transport equations. The velocities for the dislocations and disclinations with respect to the lattice have been eliminated using the energetic arguments;

- the influence of the coupling between the dislocation and disclinations have been numerically analysed in an suggestive example, which will be briefly presented.

- Within the model described by the set of equations (5.17)- (5.19), a plane edge dislocation, i.e. $\boldsymbol{\alpha} = \alpha_{13} \mathbf{e}_1 \otimes \mathbf{e}_3 + \alpha_{23} \mathbf{e}_2 \otimes \mathbf{e}_3$, coupled with wedge disclination, which is characterized by the disclination tensor $\boldsymbol{\theta} = \theta_{33} \mathbf{e}_3 \otimes \mathbf{e}_3$, has been considered. Here $\alpha_{13}, \alpha_{23}, \theta_{33}$ are functions of (x_1, x_2) only;
- the boundary of the body is free from the applied stresses and couple stresses, namely $\mathbf{T} \mathbf{n} = \mathbf{0}, \mathbf{m} \mathbf{n} = \mathbf{0}$;
- the initial condition is designed for the curvature $\boldsymbol{\kappa}^p$, i.e. $\boldsymbol{\kappa}^p(t_0) = \boldsymbol{\theta} = \theta_{33}(t_0) \mathbf{e}_3 \otimes \mathbf{e}_3$ is chosen so that to assure the compatibility with (3.23)₂, and no dislocations exist at the initial moment t_0 ;

- no yield condition has been involved in the model.

The authors mentioned that the comparison of the theoretical predictions with the experimental data and results from atomistic simulations is desirable.

5.3. Finite deformations elasto-plastic model

The following notation and definition will be used:

- the gradient of the tensorial field, say \mathbf{A} with respect to the configuration with torsion is defined in term of the gradient in the reference configuration by $\nabla_{\mathcal{K}}\mathbf{A} = (\nabla\mathbf{A})(\mathbf{F}^p)^{-1}$, $\forall\mathbf{A}$;
- ρ_0 and $\tilde{\rho}$ are mass densities in the reference and plastically deformed configurations;
- the disclination tensor pushed away to the configuration with torsion $\tilde{\mathbf{\Lambda}}$ is defined through

$$\tilde{\mathbf{\Lambda}} = \frac{1}{\det\mathbf{F}^p} \mathbf{F}^p \mathbf{\Lambda} (\mathbf{F}^p)^{-1}, \quad \tilde{\rho} \det\mathbf{F}^p = \rho_0, \quad (5.20)$$

in term of the disclination tensor in the reference configuration $\mathbf{\Lambda}$;

- the rate of disclination in the reference configuration, $\dot{\mathbf{\Lambda}}$, *pushed away* to the configuration with torsion, is considered in the model to be a measure of the variation in time of the disclination with respect to the configuration with torsion,

$$\frac{D}{Dt} \tilde{\mathbf{\Lambda}} := \frac{1}{\det\mathbf{F}^p} \mathbf{F}^p \dot{\mathbf{\Lambda}} (\mathbf{F}^p)^{-1}; \quad (5.21)$$

- three types of second order tensors will be associated with any pair \mathcal{A}, \mathcal{B} of third order tensors, following the rules written for all $\mathbf{L} \in Lin$

$$\begin{aligned} (\mathcal{A} \odot \mathcal{B}) \cdot \mathbf{L} &= \mathcal{A}[\mathbf{I}, \mathbf{L}] \cdot \mathcal{B} = \mathcal{A}_{isk} L_{sn} \mathcal{B}_{ink}, \\ (\mathcal{A} \odot_r \mathcal{B}) \cdot \mathbf{L} &= \mathcal{A} \cdot (\mathbf{L}\mathcal{B}) = \mathcal{A}_{ijk} L_{in} \mathcal{B}_{njk}, \\ (\mathcal{A} \odot_l \mathcal{B}) \cdot \mathbf{L} &= \mathcal{A} \cdot (\mathcal{B}\mathbf{L}) = \mathcal{A}_{ijk} \mathcal{B}_{ijn} L_{kn}. \end{aligned} \quad (5.22)$$

We mention that: micro force $\mathbf{\Upsilon}^p$ is power conjugate with \mathbf{L}^p ; micro momentum $\tilde{\boldsymbol{\mu}}^p$ is power conjugate with $\nabla_{\mathcal{K}}\mathbf{L}^p$; micro force $\mathbf{\Upsilon}^\lambda$ is related with the disclination mechanism, being power conjugate with the appropriate rate of $\tilde{\mathbf{\Lambda}}$, say $\frac{D}{Dt} \tilde{\mathbf{\Lambda}}$; $\tilde{\boldsymbol{\mu}}^\lambda$ is the micro stress momentum, which is power conjugated with the gradient of appropriate rate of disclination tensor, namely with $\nabla_{\mathcal{K}} \frac{D}{Dt} \tilde{\mathbf{\Lambda}}$.

The postulate of the free energy imbalance in the configuration with torsion expresses the restriction on the elasto-plastic material to be satisfied

in \mathcal{K} as an *imbalanced free energy condition*, see Cleja-Țigoiu [8], [9], as well as Gurtin et al. [22], for the initial original ideas related to the free energy imbalance. That is: the internal power has to be greater or equal to the rate of the free density energy

$$-\dot{\psi}_{\mathcal{K}} + (\mathcal{P}_{int})_{\mathcal{K}} \geq 0, \quad (5.23)$$

for an appropriate definition for the internal power $(\mathcal{P}_{int})_{\mathcal{K}}$ and for any virtual (isothermic) processes, when free energy density, $\psi_{\mathcal{K}}$, is given.

The internal power with respect to the configuration with torsion has been postulated by Cleja-Țigoiu in [8]

$$\begin{aligned} (\mathcal{P}_{int})_{\mathcal{K}} &= \frac{1}{\rho}(\mathbf{T}) \cdot \mathbf{L}^e + \frac{1}{\tilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}} \cdot \mathcal{L}_{\mathbf{L}^p}^{(e)}[\mathcal{A}_{\mathcal{K}}] + \\ &+ \frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^p \cdot \mathbf{L}^p + \frac{1}{\tilde{\rho}}\tilde{\boldsymbol{\mu}}^p \cdot \nabla_{\mathcal{K}}\mathbf{L}^p + \frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^{\lambda} \cdot \left(\frac{D}{Dt}\tilde{\boldsymbol{\Lambda}}\right) + \frac{1}{\tilde{\rho}}\tilde{\boldsymbol{\mu}}^{\lambda} \cdot \nabla_{\mathcal{K}}\frac{D}{Dt}\tilde{\boldsymbol{\Lambda}}. \end{aligned} \quad (5.24)$$

The linear operator with respect to the elastic connection $\mathcal{A}_{\mathcal{K}}^{(e)}$, dependent on the rate of plastic distortion has been introduced by Cleja-Țigoiu [8], and can be also expressed as follows

$$(\mathcal{L}_{\mathbf{L}^p}^{(e)}[\mathcal{A}_{\mathcal{K}}]) = (\mathbf{F}^e)^{-1}(\nabla_{\chi}\mathbf{L})[\mathbf{F}^e, \mathbf{F}^e] - \nabla_{\mathcal{K}}\mathbf{L}^p. \quad (5.25)$$

This formula emphasizes that the difference between the gradient of the velocity gradient, $\nabla_{\chi}\mathbf{L}$, pushed back to the configuration with torsion, and the gradient of the plastic rate calculated with respect to the configuration with torsion \mathcal{K} , is a measure for the rate elastic distortion.

Ax.1 There exists a free energy density function ψ , represented in \mathcal{K} by

$$\psi = \psi_{\mathcal{K}}(\mathbf{C}^e, \mathcal{A}_{\mathcal{K}}^{(e)}, (\mathbf{F}^p)^{-1}, \mathcal{A}_{\mathcal{K}}^{(p)}, \tilde{\boldsymbol{\Lambda}}, \nabla_{\mathcal{K}}\tilde{\boldsymbol{\Lambda}}). \quad (5.26)$$

The axiom asserts that the free energy density function is dependent on:

- the second order elastic deformation $(\mathbf{C}^e, \mathcal{A}_{\mathcal{K}}^{(e)})$, were $\mathbf{C}^e = (\mathbf{F}^e)^T\mathbf{F}^e$ and $\mathcal{A}_{\mathcal{K}} = (\mathbf{F}^e)^{-1}\nabla_{\mathcal{K}}\mathbf{F}^e$;

- the plastic measure of deformation $((\mathbf{F}^p)^{-1}, \mathcal{A}_{\mathcal{K}}^{(p)})$, where the expression of the Bilby type plastic connection $\mathcal{A}_{\mathcal{K}}^{(p)}$ is related to $\mathcal{A}^{(p)}$ by

$$\mathcal{A}_{\mathcal{K}}^{(p)} = -\mathbf{F}^p \mathcal{A}^{(p)} [(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}]; \quad (5.27)$$

- the disclination variable $\tilde{\boldsymbol{\Lambda}}$ and its gradient in \mathcal{K} .

Based on the above introduced definitions it can be proved the following proposition.

Proposition 5.1. *The equivalent expression of the free energy density (5.26) can be written in terms of the appropriate fields with respect to the reference configuration*

$$\psi = \psi(\mathbf{C}, \boldsymbol{\Gamma}, \mathbf{F}^p, \overset{(p)}{\mathcal{A}}, \boldsymbol{\Lambda}, \nabla \boldsymbol{\Lambda}). \quad (5.28)$$

Ax.2 The micro balance equation for micro forces associated with the disclination are postulated to satisfy their own balance equations

$$\boldsymbol{\Upsilon}^\lambda = \operatorname{div}_{\mathcal{K}} \boldsymbol{\mu}^\lambda + \tilde{\rho} \mathbf{B}^\lambda \iff J^p \boldsymbol{\Upsilon}^\lambda = \operatorname{div} (J^p \boldsymbol{\mu}^\lambda (\mathbf{F}^p)^{-T}) + \tilde{\rho} \mathbf{B}^\lambda,$$

$$J^p = | \det \mathbf{F}^p |.$$

Ax.3 The micro balance equation for micro forces associated with the irreversible behaviour is expressed through

$$\boldsymbol{\Upsilon}^p = \operatorname{div}_{\mathcal{K}} (\boldsymbol{\mu}^p) + \tilde{\rho} \mathbf{B}^\lambda \iff$$

$$J^p \boldsymbol{\Upsilon}^p = \operatorname{div} (J^p (\boldsymbol{\mu}^p) (\mathbf{F}^p)^{-T}) + \tilde{\rho} \mathbf{B}^p.$$

Thermomechanical restrictions can be derived from the imbalance free energy postulate, when we suppose that the plastic and disclination mechanism is frozen. These restrictions can be summarized as follows:

1. the free energy density is potential for the symmetric part of the Cauchy stress tensor and for the macro momentum, written in the reference configuration

$$\frac{1}{\hat{\rho}} \{\boldsymbol{\Gamma}\}^s = 2\mathbf{F}(\partial_{\mathbf{C}}\psi)\mathbf{F}^T, \quad \frac{1}{\rho_0} \boldsymbol{\mu}_0 = \partial_{\boldsymbol{\Gamma}}\psi; \quad (5.29)$$

2. the free energy density is potential for the micro stress momenta,

$$\frac{1}{\rho_0} \boldsymbol{\mu}_0^p = \partial_{\overset{(p)}{\mathcal{A}}}\psi, \quad \frac{1}{\rho_0} \boldsymbol{\mu}_0^\lambda = \partial_{\nabla \boldsymbol{\Lambda}}\psi^d(\nabla \boldsymbol{\Lambda}), \quad (5.30)$$

where $\boldsymbol{\mu}_0^p, \boldsymbol{\mu}_0^\lambda$ represent the plastic micro momentum and the micro momentum related with the disclination mechanism;

3. the viscoplastic type equations which establish the relationships for the variation in time of plastic distortion and of the disclination tensor have been expressed (that is the appropriate evolution equations)

$$\begin{aligned} \xi_1 \dot{\mathbf{I}}^p &= \frac{1}{\rho_0} (\boldsymbol{\Sigma}_0 - \boldsymbol{\Sigma}_0^p) + (\mathbf{F}^p)^T \partial_{\mathbf{F}^p} \psi, \quad \mathbf{I}^p = -(\mathbf{F}^p)^{-1} \dot{\mathbf{F}}^p, \\ \xi_3 \dot{\boldsymbol{\Lambda}} &= \left(\frac{1}{\rho_0} \boldsymbol{\Sigma}_0^\lambda - \partial_{\boldsymbol{\Lambda}} \psi \right) + \left(\overset{(p)}{\mathcal{A}} \odot \frac{1}{\rho_0} \boldsymbol{\mu}_0^\lambda \right) - \\ &\quad - \left(\frac{1}{\rho_0} \boldsymbol{\mu}_0^\lambda \text{ }_r \odot \overset{(p)}{\mathcal{A}} \right) - \frac{1}{\rho_0} \boldsymbol{\mu}_0^\lambda (\operatorname{tr}_{(2)}(\overset{(p)}{\mathcal{A}})); \end{aligned} \quad (5.31)$$

4. the expression of the resulting reduced dissipation inequality can be finally written $\xi_1 \mathbf{P} \cdot \mathbf{P} + \xi_3 \dot{\mathbf{A}} \cdot \dot{\mathbf{A}} \geq 0$.

Here $\Sigma_0, \Sigma_0^p, \Sigma_0^\lambda$ are Mandel's type stress measures, written in the reference configuration, defined in terms of the Cauchy stress \mathbf{T} , micro forces Υ^p and Υ^λ , respectively, as it follows

$$\begin{aligned} \frac{1}{\rho_0} \Sigma_0 &= \mathbf{F}^T \frac{1}{\rho} \mathbf{T} \mathbf{F}^T, & \Sigma_0^p &= \frac{1}{\tilde{\rho}} (\mathbf{F}^p)^T \Upsilon^p (\mathbf{F}^p)^{-T}, \\ \Sigma_0^\lambda &= \frac{1}{\tilde{\rho}} (\mathbf{F}^p)^T \Upsilon^\lambda (\mathbf{F}^p)^{-T}. \end{aligned} \tag{5.32}$$

The plastic micro momentum, the micro momentum related with the disclination mechanism, and the macro momentum relative to the reference configuration are defined by

$$\begin{aligned} \frac{1}{\rho_0} \boldsymbol{\mu}_0^p &:= (\mathbf{F}^p)^T \frac{1}{\tilde{\rho}} \tilde{\boldsymbol{\mu}}^p [(\mathbf{F}^p)^{-T}, (\mathbf{F}^p)^{-T}], \\ \frac{1}{\rho_0} \boldsymbol{\mu}_0^\lambda &:= (\mathbf{F}^p)^T \frac{1}{\tilde{\rho}} \tilde{\boldsymbol{\mu}}^\lambda [(\mathbf{F}^p)^{-T}, (\mathbf{F}^p)^{-T}], & \frac{1}{\rho_0} \boldsymbol{\mu}_0 &:= \mathbf{F}^T \frac{1}{\tilde{\rho}} \boldsymbol{\mu}_K [\mathbf{F}^{-T}, \mathbf{F}^{-T}]. \end{aligned} \tag{5.33}$$

6. Conclusions

The *plastic deformability of metals*, which are crystalline materials, is produced due to the *existence of lattice defects inside the micro structure*. The *dislocations, disclinations* and *point defects* are viewed as defects and were mathematically modeled by the *differential geometry concepts* as torsion, curvature and measure of non-metricity, in the case of continuously distributed defects. The linear approximation of the continuum theory of lattice defects within the non-Euclidean geometry has been proposed by de Wit [17]. There are different, independent ways from the geometrical point of view in defining the two types of defects, dislocations and disclinations, which may or may not be related to each other, and which lead to completely different mathematical descriptions or theories.

The presence of the Burgers and Frank vectors is the starting point in constructing the dislocations and disclinations models and make the differences between them.

As for instance, the elastic models for defects are built

- by solving the elasticity problem in multiply-connected domain, where the compatibility conditions (see section3) are satisfied;
- by solving the elastic problems in simply connected domain, which contains the cut surface on which the jump conditions (see section3) are written in terms of constants, which means Burgers' and Frank's vectors;

The appropriate elastic type problems are solved without any specification of the nature of the defects involved in the models.

The elasto-plastic model with small strains, shortly presented in sections 5.2, 5.3, stipulate evolution equations for plastic fields and for incompatibilities (identified with the measure for the defects), while the balance equations for macro forces (say stress and couple stresses) are satisfied by the elastic type constitutive equations. The solutions have no singularities, although the elastic and plastic strains (and curvatures) are incompatible, the displacement vectors and the rotation vectors follow to be well defined.

We described the behaviour of an elasto-plastic material with structural defects, undergoing finite deformations, based on the *existence of time dependent configurations with torsion*. The configuration with torsion is viewed like a second order deformation, namely a pair of a second order tensor, called *plastic distortion* and *plastic connection with torsion*. The presence of the (physical) defects means from the mathematical point of view the non-zero torsion and non-zero curvature of the plastic connection. The energetic arguments, like the macro and micro balance equations and the energy imbalance principle, are extended to incorporate the dissipated power during the irreversible behaviour cumulated by the developed defect mechanism as well as by the plastic mechanism. The thermomechanical restrictions on the constitutive functions have been obtained under the form of the elastic type constitutive equations, which satisfy the balance equations for macro forces (stress and couple stresses). Through the appropriate (non-local) evolution equations which are compatible with the reduced dissipation inequality, the microstructural defects are related with macroscopic and microscopic forces, which satisfy the appropriate balance equations. The initial and boundary value problems are formulated to complete the models. In this paper we presented a possible approach to finite elasto-plastic model for crystalline materials with microstructural defects.

We can associate the model, which describes the behaviour of an elasto-plastic material with structural defects undergoing finite deformations, with a model involving small elastic and plastic distortions. In such a way we could validate the finite deformation model by making comparison between the already known results obtained within small deformations models and those derived for the associated model. As for instance, the formulae which characterize the framework of second order finite elasto-plasticity with the plastic connection having metric property, allow us to introduce the measure of the dislocation and to prove the existence of a second order tensor, the disclination tensor $\mathbf{\Lambda}$, which leads to a non-vanishing curvature, namely to a non-zero Frank vector, under the hypothesis of small elasto-plastic distortions. We obtain appropriate evolution equations for the plastic distortion and for the disclination tensor. To describe the influence of the coupling between the dislocation and disclinations on the behaviour of an elasto-plastic material with structural defects, first the initial and boundary value problem must be formulated. Second the particular cases of wedge disclination

and edge dislocation must be analysed, following physical description of the model given in [19].

The comparison of the theoretical predictions with the experimental data and results from atomistic simulations ought to be desirable.

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