Arch Appl Mech (2014) 84:1293–1306
DOI 10.1007/s00419-014-0913-3

SPECIAL

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Dislocations and disclinations: continuously distributed defects in elasto-plastic crystalline materials

Received: 6 June 2014 / Accepted: 21 August 2014 / Published online: 12 October 2014

Abstract The paper deals with elasto-plastic models for crystalline materials with defects, dislocations coupled with disclinations. The behaviour of the material is described with respect to an anholonomic configuration, endowed with a non-Riemannian geometric structure. The geometry of the material structure is generated by the plastic distortion, which is an incompatible second-order tensor, and by the so-called plastic connection which is metric compatible, with respect to the metric tensor associated with the plastic distortion. The free energy function is dependent on the second-order elastic deformation and on the state of defects. The tensorial measure of the defects is considered to be the Cartan torsion of the plastic connection and the disclination tensor. When we restrict to small elastic and plastic distortions, the measures of the incompatibility as well as the dislocation densities reduced to the classical ones in the linear elasticity. The constitutive equations for macroforces and the evolution equations for the plastic distortion and disclination tensor are provided to be compatible with the free energy imbalance principle.

Keywords Dislocation and disclination densities · Torsion and curvature of plastic connection · Viscoplastic constitutive equations · Free energy imbalance principle

1 Introduction

The paper deals with elasto-plastic models for crystalline materials with defects, such as dislocations coupled with disclinations. The attention is focused on the description of the structural defects in terms of the fields which characterize the irreversible behaviour of the material, via the evolution equations within the second-order finite elasto-plasticity provided by Cleja-Ţigoiu [10,11].

The elastic models for dislocations and disclinations have been obtained within the linear theory of elasticity and the solutions undergo discontinuities at the dislocation and disclination lines, respectively. de Wit [17,18] and Kossecka and de Wit [25] mean by defects the combination of dislocations and disclinations by the word defect, and refer to the strain and bent-twist as the basic fields. The problems formulated by de Wit [18] and Kossecka and de Wit [25] concern the finding of the elastic basic fields and the stress, when the basic plastic fields, or the defect densities, for the dislocations, $\boldsymbol{\alpha}$, and for disclinations, $\boldsymbol{\omega}$, are prescribed (without specifying the nature of these defects), see also Mura [35]. The incompatibilities in linear elasticity were reviewed by de Wit [15,19], Kossecka and de Wit [25] and Fressengeas et al. [22]. The differential operators of higher orders of the elastic strain were introduced, and using the gradient modified elastic law, the singularities in the strain

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and stress were eliminated from the description of the dislocations and disclinations, see for instance Gutkin and Aifantis [24], Lazar et al. [28] and Deng et al. [14].

Disclinations have been illustrated similarly to dislocations based on the Volterra description, see de Wit [18]. An uniform and isotropic elastic hollow cylinder is cut, the two shores of the cut-off surface are rotated (disclinations) instead of the translated (dislocations) relative to each other. The strength of dislocation is determined by Burgers vector, **b**, which is equal to the translational displacement, and in a similar way, the strength of disclination is determined by Frank vector, $\boldsymbol{\Omega}$, which is equal to the rotational displacement, see [16,18] and [25]. In [17], de Wit proved that is not possible to have a disclination theory without dislocations, but a pure dislocation theory can be constructed within the small strain framework.

The physical examples of the rotational defect structures related to disclinations can be observed in crystalline materials as have been presented by Romanov [37] and Romanov and Kolesnikova [38]. The transmission electron microscopy emphasized the occurrence of self-organized structures, ladder-like structure or persistent slip bands which evolve. "Disclinations, as a second kind of deformation carrying defects, are especially adapted to rotational modes and to the mesoscopic structural levels, while the dislocations are especially adapted to translational modes and to the microstructure", as it is noticed by Seefeldt and Klimanek [40]. The microstructural features of the deformed single crystals in terms of the *global average densities* of dislocations and disclinations and the contribution of the mentioned defects to flow stress are considered by Seefeldt and Klimanek [40,41], Romanov [37] and Walgraef and Aifantis [44,45] (for the dislocations only).

The various elastic models for dislocations were developed by Teodosiu [43], to find the displacement vector as an uniform function which has given discontinuities (compatible with Burgers vector) on the cut-off surfaces in the domain occupied by the body. The internal mechanical state of solids with defects leads Kröner [26] and [27], to solve the elastic problems with given incompatibilities and to introduce the definitions of the defects, as dislocations and disclinations, based on differential geometric concepts related to the connection which are or not compatible with the appropriate metric tensor.

The attempts to modify the elastic fields of these defects were done by considering the couple stresses within the Cosserat continuum and in micropolar materials. Mayeur et al. [32] proposed an elasto-plastic model involving a continuum measure of the deformation incompatibility, the so-called geometrically necessary dislocation (GND) density tensor $\boldsymbol{\alpha}$. The GND density tensor $\boldsymbol{\alpha}$ is decomposed in the appropriate edge and screw dislocations, as in Arsenlis and Parks [2]. The scalar GND densities in the slip system α, $\rho^{\alpha}_{G,\perp}$ and $\rho^{\alpha}_{G,\parallel}$, are defined *as gradients of shear slip projected in the glide directions for pure edge and screw dislocations*. The microstructural evolution is related also to the change in the *statistically stored dislocation*, which evolves as described by Kocks-Mecking in [34]. The evolution equations for the plastic distortion, $\mathbf{H}^p$, is like in crystal plasticity, while the torsion-curvature tensor, $\boldsymbol{\kappa}^p$, evolves following the appropriate slip directions. In the models developed for instance in Arsenlis and Parks [2], Cermelli and Gurtin [4], Gurtin et al. [23], the Burgers vector has been defined by the GND-tensor $\mathbf{F}^p\mathrm{curl}\mathbf{F}^p$ in the lattice space.

Fressengeas et al. [22] aim to present a *field defect* (dislocation and disclination) theory for crystal plasticity accounting for both the translational and rotational aspects of lattice incompatibility. The authors restricted to small strain framework and proved that the proposed model reduces to field dislocation mechanics when the disclination density vanishes. The constitutive relationships provide the non-symmetric Cauchy stress, **T**, and couple-stress tensor, **m**, in terms of elastic strain and bent-twist, $\boldsymbol{\varepsilon}^e$ and $\boldsymbol{\kappa}^p$. The macroforces, **T** and **m**, satisfy the balance equation formulated by Fleck et al. [21]. The evolution equations for basic plastic fields, $\boldsymbol{\varepsilon}^p$, $\boldsymbol{\kappa}^p$, are dependent on the density of dislocations and disclinations, $\boldsymbol{\alpha}$ and $\boldsymbol{\theta}$, and on macroforces. In order to solve the elasto-plastic problem, the initial and boundary conditions have to be considered. The boundary conditions prescribe the stress and couple-stress tensors (i.e. macroforces) or the displacement and rotation on the surface of the body. The microboundary conditions for modelling the interfaces have also to be considered: as for instance, the *microhard* condition to represent the case where dislocations are *blocked*, and *microfree* condition to represent the case where dislocations are *unobstructed at the interface* (see Mayeur and McDowel [33]). Fressengeas et al. [22] considered that the dislocation and disclination densities have to be specified on *inflow* boundary, but no condition is required on the outflow boundaries.

In this paper, we describe the behaviour of elasto-plastic materials with structural defects, undergoing finite deformations, based on the existence of time-dependent anholonomic configurations, the so-called configurations with torsion, following the constitutive framework developed by Cleja-Ţigoiu [10,11]. The constitutive framework developed here attempt to clarify both questions formulated by Le and Günther [29] concerning (i) the kinematical-independent and kinematical-dependent quantities, which characterize the state of crystals with defects and their evolution equations, (ii) the specification of the free energy density and the dissipation within the adopted constitutive framework.

The macroforces, $\mathbf{T}$ which is non-symmetric Cauchy stress, and $\boldsymbol{\mu}$ which represents the macrostress momentum (a third-order tensor) satisfy the local balance law for linear momentum equation in the deformed configuration of the body, written under the form

$$\operatorname{div}\left(\mathbf{T}^s - \frac{1}{2}\{\operatorname{div}\boldsymbol{\mu}\}^a\right) + \rho\mathbf{b} = \rho\mathbf{a}. \tag{1}$$

This form is provided by Cleja-Ţigoiu and Ţigoiu [9], following Fleck et al. [21].

The microforces, i.e. microstress and microstress momentum, which generate internal power satisfy their appropriate microbalance equations, see for instance [12]. The constitutive and evolution equations for plastic distortion and disclination tensor are derived to be compatible with the free energy imbalance principle. We adapted to the second-order finite elasto-plasticity in [10,11] the free energy imbalance principle previously provided in global and local forms within elasto-plastic materials by Gurtin et al. [23].

1.1 List of notations

Further the following notations will be used:
$\mathcal{E}$—the three-dimensional Euclidean space, with the vector space of translations $\mathcal{V}$; Lin—the set of the linear mappings from $\mathcal{V}$ to $\mathcal{V}$, i.e the set of second-order tensor, $Skew \subset$ Lin the set of all skew-symmetric second-order tensors;

$\mathbf{u}\cdot\mathbf{v}, \mathbf{u}\times\mathbf{v}, \mathbf{u}\otimes\mathbf{v}$ 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
$(\mathbf{a}\otimes\mathbf{b})\mathbf{u} = \mathbf{a}(\mathbf{b}\cdot\mathbf{u}), \quad (\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c})\mathbf{u} = (\mathbf{a}\otimes\mathbf{b})(\mathbf{c}\cdot\mathbf{u}), \quad$ for all vectors $\mathbf{u}$.
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;
definition of the trace: $\operatorname{tr}\mathbf{A}((\mathbf{u}\times\mathbf{v})\cdot\mathbf{z}) = (\mathbf{A}\mathbf{u},\mathbf{v},\mathbf{z}) + (\mathbf{u},\mathbf{A}\mathbf{v},\mathbf{z}) + (\mathbf{u},\mathbf{v},\mathbf{A}\mathbf{z})$;
definition of the adjoint: $(\mathbf{A}\mathbf{u},\mathbf{A}\mathbf{v},\mathbf{z}) = (\mathbf{u},\mathbf{v},(\operatorname{Adj}\mathbf{A})\mathbf{z})$;
the tensorial product $\mathbf{A}\otimes\mathbf{a}$ for $\mathbf{a}\in\mathcal{V}$, is a third-order tensor, with the property
$(\mathbf{A}\otimes\mathbf{a})\mathbf{v} = \mathbf{A}(\mathbf{a}\cdot\mathbf{v}), \forall\mathbf{v}\in\mathcal{V}$.

$\mathbf{I}$ is the identity tensor in Lin, and $\mathbf{A}^T$ denotes the transpose of $\mathbf{A}\in$ Lin,
$\partial_{\mathbf{A}}\phi(x)$ denotes the partial differential of the function ϕ with respect to the field $\mathbf{A}$.
Curl of a second-order tensor field $\mathbf{A}$ is defined by the second-order tensor field

$$(\operatorname{curl}\mathbf{A})(\mathbf{u}\times\mathbf{v}) := (\nabla\mathbf{A}(\mathbf{u}))\mathbf{v} - (\nabla\mathbf{A}(\mathbf{v}))\mathbf{u} \quad \forall\mathbf{u},\mathbf{v}\in\mathcal{V}. \tag{2}$$

Remark 1.1 The component of curl$\mathbf{A}$ given in a Cartesian basis are defined by

$$(\operatorname{curl}\mathbf{A})_{pi} = \epsilon_{ijk}\frac{\partial A_{pk}}{\partial x^j},$$

but curl of $\mathbf{F}^p$ is taken in $\mathcal{B}$ and the basis is $\{\mathbf{G}_j\}$.

In what follows, the following definitions and notation will be useful:

Definition 1.1 For any $\boldsymbol{\Lambda}_1, \boldsymbol{\Lambda}_2\in$ Lin we define a third-order tensor associated with them, denoted $\boldsymbol{\Lambda}_1\times\boldsymbol{\Lambda}_2$, by

$$((\boldsymbol{\Lambda}_1\times\boldsymbol{\Lambda}_2)\mathbf{u})\mathbf{v} = (\boldsymbol{\Lambda}_1\mathbf{u})\times(\boldsymbol{\Lambda}_2\mathbf{v}), \quad \forall\ \mathbf{u},\mathbf{v}. \tag{3}$$

Definition 1.2 The *Adjoint* of $\widetilde{\boldsymbol{\Lambda}}$, denoted by $Adj(\widetilde{\boldsymbol{\Lambda}})$, is *the second-order tensor* defined by

$$\left(\widetilde{\boldsymbol{\Lambda}}\mathbf{u},\widetilde{\boldsymbol{\Lambda}}\mathbf{v},\mathbf{w}\right) := \left(\mathbf{u},\mathbf{v},(Adj\ \widetilde{\boldsymbol{\Lambda}})\mathbf{w}\right), \quad \forall\ \mathbf{u},\mathbf{v},\mathbf{w}. \tag{4}$$

Let us introduce three types of second-order tensors that can be associated with any pair of third-order tensors, $\mathcal{A}$, $\mathcal{B}$, following the rules written below

$$(\mathcal{A} \odot \mathcal{B}) \cdot \mathbf{L} = \mathcal{A}[\mathbf{I}, \mathbf{L}] \cdot \mathcal{B} = \mathcal{A}_{isk} L_{sn} \mathcal{B}_{ink}$$
$$(\mathcal{A}\,_r \odot \mathcal{B}) \cdot \mathbf{L} = \mathcal{A} \cdot (\mathbf{L}\mathcal{B}) = \mathcal{A}_{ijk} L_{in} \mathcal{B}_{njk} \tag{5}$$
$$(\mathcal{A} \odot_l \mathcal{B}) \cdot \mathbf{L} = \mathcal{A} \cdot (\mathcal{B}\mathbf{L}) = \mathcal{A}_{ijk} \mathcal{B}_{ijn} L_{kn}.$$

for all $\mathbf{L} \in \mathrm{Lin}$.

Notation 1.1 For any third-order field, say $\mathcal{N}$, we denote by $Skw\mathcal{N}$ the third-order tensor which has the property

$$((Skw\mathcal{N})\mathbf{u})\mathbf{v} = (\mathcal{N}\mathbf{u})\mathbf{v} - (\mathcal{N}\mathbf{v})\mathbf{u}, \quad \forall \quad \mathbf{u}, \mathbf{v}. \tag{6}$$

Let us introduce the following notation $\mathcal{A}[\mathbf{F}_1, \mathbf{F}_2]$ for the field generated by a third-order tensor $\mathcal{A}$ and the second-order tensors, for instance $\mathbf{F}_1$, $\mathbf{F}_2$, which is defined by

$$((\mathcal{A}[\mathbf{F}_1, \mathbf{F}_2])\mathbf{u})\mathbf{v} = (\mathcal{A}(\mathbf{F}_1\mathbf{u}))\mathbf{F}_2\mathbf{v} \tag{7}$$

for all vectors $\mathbf{u}$, $\mathbf{v}$. $\mathcal{B}$ denotes the elasto-plastic body considered to be a material manifold. $\mathbf{X} \in \mathcal{B}$ is a material point, and χ is the function which defines the motion of the body $\mathcal{B}$.

2 Measures of dislocations and disclinations

If there are defects inside the body, a global stress-free configuration does not exists (Mandel [30], Teodosiu [42], Cleja-Ţigoiu and Sóos [8]) and the geometry of the material structure with defects can be characterized by anholonomic configurations (see Schouten [39], Acharya and Bassani [1], Clayton et al. [6]). In the paper by Clayton [7], the concepts of anholonomic geometry are refined and extended to the so-called intermediate configuration, previously used within the context of crystalline solids with continuously distributed dislocation [6] and [5]. Although even a global stress-free configuration does not exists, it is possible to locally relax the neighbourhoods of the material points in which the body $\mathcal{B}$ can be divided. These relaxed neighbourhoods become incompatible, and they cannot fit together. Yavari [47] presented the background of the Riemann–Cartan geometry which allow to describe continuously distributed defects in solids.

The behaviour of elasto-plastic body, $\mathcal{B}$, (a material manifold) is characterized with respect to the so-called configuration with torsion, $\mathcal{K}$, which is an anholonomic configuration associated with the material manifold. The geometry of the configuration with torsion is characterized by the second-order pair of plastic deformation, which consists of

- the plastic distortion, $\mathbf{F}^p$, which is an incompatible or non-integrable field, that means $\mathrm{curl}\mathbf{F}^p \neq 0$, and
- the so-called plastic connection, $\overset{(p)}{\mathbf{\Gamma}}$, which has nonzero torsion and nonzero curvature.

The plastic connection on the body manifold $\mathcal{B}$ is a linear (affine) connection, $\overset{(p)}{\nabla}: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \longrightarrow \mathcal{X}(\mathcal{B})$, where $\mathcal{X}(\mathcal{B})$ is the set of vector field on $(\mathcal{B})$ (see [47]), which is denoted here by $\overset{(p)}{\mathbf{\Gamma}}$.

We mention two basic hypotheses put down on the background of the constitutive framework:

- the **first incompatibility condition**, i.e. the plastic distortion has non-vanishing *curl*, $curl(\mathbf{F}^p) \neq 0$, which means that the plastic distortion cannot be expressed through the gradient of a certain vector field, apart from the deformation gradient, $\mathbf{F} = \nabla\chi(\mathbf{X}, t)$;
- the **second integrability condition,** i.e. the plastic connection has nonzero curvature, which means that $\overset{(p)}{\mathbf{\Gamma}}$ is not compatible with plastic distortion, i.e. $\overset{(p)}{\mathbf{\Gamma}} \neq (\mathbf{F}^p)^{-1}\, \nabla(\mathbf{F}^p)$.

We assume that the connection $\overset{(p)}{\boldsymbol{\Gamma}}$ is *metric compatible* with respect to the metric tensor $\mathbf{C}^p$, induced by the plastic distortion, namely $\mathbf{C}^p = (\mathbf{F}^p)^T\mathbf{F}^p$. Generally, the connection is related to crystallographic lattice and can have nonzero torsion and characterizes the dislocation density (see Kröner [26] and [27]) or the inhomogeneity (see Noll [36], Epstein and Maugin [20]).

We recall our basic relationships which characterize the elasto-plastic material from the geometrical point of view.

The *multiplicative decomposition* of the deformation gradient $\mathbf{F}$ into its elastic and plastic components, $\mathbf{F}^e$ and $\mathbf{F}^p$, called distortions, namely

$$\mathbf{F} = \mathbf{F}^e\mathbf{F}^p, \quad \Longleftrightarrow \quad \mathbf{F}^e = \mathbf{F}(\mathbf{F}^p)^{-1}, \tag{8}$$

holds. The deformation gradient is expressed in coordinate systems by

$$\mathbf{F}(\mathbf{X}, t) = \nabla\chi(\mathbf{X}, t) = \frac{\partial x^i}{\partial X^j}\mathbf{g}_i \otimes \mathbf{G}^j. \tag{9}$$

The differential of smooth field $\mathbf{A}$, with respect to the anholonomic configuration $\mathcal{K}$, obeys the rule

$$\nabla_{\mathcal{K}}\mathbf{A} = (\nabla\mathbf{A})(\mathbf{F}^p)^{-1}. \tag{10}$$

In what follows, the anholonomic basis vectors are related to *the crystal* and is defined by $\mathbf{e}_j = \mathbf{F}^p\mathbf{G}_j$. The Christoffel symbols $[\,\overset{(p)}{\boldsymbol{\Gamma}}\,]^i\mathbf{G}_i$ of the plastic connection are represented by

$$\overset{(p)}{\boldsymbol{\Gamma}}(\mathbf{G}_j, \mathbf{G}_k) = [\,\overset{(p)}{\Gamma}\,]^i_{jk}\mathbf{G}_i. \tag{11}$$

The motion of the body, χ, induces a second-order pair of deformation which is defined by $(\mathbf{F}, \boldsymbol{\Gamma} := (\mathbf{F})^{-1}(\nabla\mathbf{F}))$. $\boldsymbol{\Gamma}$ is called the motion connection. If we accept the existence of the plastic connection, then there exists a second-order pair, the so-called *elastic second-order deformation*, $(\mathbf{F}^e, \overset{(e)}{\boldsymbol{\Gamma}}_{\mathcal{K}})$, satisfying the relation (8) and the transformation rule of the connections, i.e. *the connections* $\boldsymbol{\Gamma}$, $\overset{(e)}{\boldsymbol{\Gamma}}_{\mathcal{K}}$ and $\overset{(p)}{\boldsymbol{\Gamma}}$ are related by

$$\boldsymbol{\Gamma} = (\mathbf{F}^p)^{-1}(\overset{(e)}{\boldsymbol{\Gamma}}_{\mathcal{K}}[\mathbf{F}^p, \mathbf{F}^p]) + \overset{(p)}{\boldsymbol{\Gamma}}. \tag{12}$$

The transformation rule (12) generalized the composition rule for the second-order gradients given by Cross [13] and Wang [46], and was called composition rule of connections.

In Cleja-Ţigoiu [11], the following propositions have been proved.

Proposition 2.1 *Under the hypothesis concerning the composition of the connection* (12) *together with the multiplicative decomposition of* $\mathbf{F}$*, postulated in* (8)*, we get*

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

$\overset{(e)}{\mathcal{A}}_{\mathcal{K}}$ *and* $\overset{(p)}{\mathcal{A}}$ *define the Bilby-type connection (see Bilby [3]) with respect to the configuration with torsion and initial one, respectively.*

2.1 Plastic connection with metric property

Let us introduce the metric tensor $\mathbf{C}^p = (\mathbf{F}^p)^T \mathbf{F}^p$ generated by $\mathbf{F}^p$.

Proposition 2.2 *The plastic connection, which is metric compatible with respect to the metric tensor $\mathbf{C}^p$, is represented by Cleja-Ţigoiu [11] under the form*

$$\overset{(p)}{\mathbf{\Gamma}} = \overset{(p)}{\mathcal{A}} + (\mathbf{C}^p)^{-1} (\mathbf{\Lambda} \times \mathbf{I}), \tag{14}$$

where the third-order tensor $\mathbf{\Lambda} \times \mathbf{I}$ is generated by the second-order (covariant) tensor $\mathbf{\Lambda}$ and is defined by (3). $\mathbf{\Lambda}$ is called the disclination tensor.

Definition 2.1 The Cartan torsion associated with the plastic connection $\overset{(p)}{\mathbf{\Gamma}}$ is defined as

$$\mathbf{S}^p(\mathbf{u}, \mathbf{v}) = \overset{(p)}{\mathbf{\Gamma}} (\mathbf{u}, \mathbf{v}) - \overset{(p)}{\mathbf{\Gamma}} (\mathbf{v}, \mathbf{u}) - [\mathbf{u}, \mathbf{v}], \tag{15}$$

where $[\mathbf{u}, \mathbf{v}]$ represents the Lie brackets of the vectors $\mathbf{u}$ and $\mathbf{v}$.

In a given coordinate system, the components of the Cartan torsion, which is a third-order tensor, are equivalently given by

$$(S^p)^i{}_{jk} = [\overset{(p)}{\Gamma}]^i_{jk} - [\overset{(p)}{\Gamma}]^i_{kj}. \tag{16}$$

The non-vanishing torsion of the plastic connection can be considered to be a measure for the *incompatibility of plastic deformation.*

Proposition 2.3 *The second-order torsion tensor $\mathcal{N}^p$ is associated with Cartan torsion (15) and is expressed by*

$$\begin{aligned} &\mathcal{N}^p = (\mathbf{F}^p)^{-1} curl \mathbf{F}^p + (\mathbf{C}^p)^{-1} \big((tr\, \mathbf{\Lambda})\mathbf{I} - (\mathbf{\Lambda})^T\big), \\ &where \quad \mathbf{S}^p(\mathbf{u}, \mathbf{v}) = \mathcal{N}^p(\mathbf{u} \times \mathbf{v}). \end{aligned} \tag{17}$$

2.2 Measure of disclinations

The disclination tensor with respect to the configuration with torsion will be denoted by $\widetilde{\mathbf{\Lambda}}$ and is associated with the second-order tensor $\mathbf{\Lambda}$, see Cleja-Ţigoiu [11].

Proposition 2.4 *If $\overset{(p)}{\mathbf{\Gamma}}$ has metric property, then the elastic connection with respect to the configuration with torsion allows a representation given by*

$$\begin{aligned} &\overset{(e)}{\mathbf{\Gamma}}_{\mathcal{K}} = \overset{(e)}{\mathcal{A}}_{\mathcal{K}} - (\mathbf{F}^p)^{-T} (\mathbf{\Lambda} \times \mathbf{I})[(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}], \quad or \\ &\overset{(e)}{\mathbf{\Gamma}}_{\mathcal{K}} = \overset{(e)}{\mathcal{A}}_{\mathcal{K}} - \widetilde{\mathbf{\Lambda}} \times \mathbf{I}, \end{aligned} \tag{18}$$

where the measure of the disclination, viewed in the configuration with torsion $\mathcal{K}$, can be introduced through

$$\begin{aligned} &\widetilde{\mathbf{\Lambda}} = \frac{1}{det \mathbf{F}^p} \mathbf{F}^p \mathbf{\Lambda} (\mathbf{F}^p)^{-1}, \quad \widetilde{\rho} det \mathbf{F}^p = \rho_0, \ or \\ &(\mathbf{F}^p)^{-T} (\mathbf{\Lambda} \times \mathbf{I})[(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}] = \widetilde{\mathbf{\Lambda}} \times \mathbf{I}. \end{aligned} \tag{19}$$

Proof If we consider the relationships (12) and (13) together with (14), the first expression written in (18) follows at once.

Let us find the relationship between two fields $\widetilde{\mathbf{\Lambda}}$ and $\mathbf{\Lambda}$, which obeys the rule

$$(\widetilde{\mathbf{\Lambda}}\tilde{\mathbf{u}} \times \tilde{\mathbf{v}}) \cdot \tilde{\mathbf{z}} = (\mathbf{\Lambda u} \times \mathbf{v}) \cdot \mathbf{z}, \tag{20}$$

written for all $\tilde{\mathbf{z}}$ and $\mathbf{z}$ related by $\tilde{\mathbf{z}} = \mathbf{F}^p\mathbf{z}$.

On the one hand, the left-hand side in (20) can be transformed in

$$(\widetilde{\mathbf{\Lambda}}\tilde{\mathbf{u}} \times \tilde{\mathbf{v}}) \cdot \tilde{\mathbf{z}} = \widetilde{\mathbf{\Lambda}}(\mathbf{F}^p\mathbf{u}) \cdot (\mathbf{F}^p\mathbf{v} \times \mathbf{F}^p\mathbf{z}) \tag{21}$$

and on the other hand, using the definition of the determinant written for $\mathbf{F}^p$, the following identity holds

$$\mathbf{F}^p\mathbf{u} \times \mathbf{F}^p\mathbf{v} = \det\mathbf{F}^p \ (\mathbf{F}^p)^{-T}(\mathbf{u} \times \mathbf{v}), \ \forall \ \mathbf{u}, \mathbf{v}. \tag{22}$$

As a consequence of the relationships (21) and (22), the equality (20) holds if and only if

$$\mathbf{\Lambda} = \det\mathbf{F}^p(\mathbf{F}^p)^{-1}\widetilde{\mathbf{\Lambda}}\mathbf{F}^p. \tag{23}$$

We define *Burgers and Frank vectors* in terms of the plastic distortion $\mathbf{F}^p$ and disclination tensor $\widetilde{\mathbf{\Lambda}}$. Both vectors are associated with a circuit C_0 in the reference configuration, being represented in terms of the dislocation and disclinations densities defined in the configuration with torsion.

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

Proposition 2.5 *Let the curvature tensor that belongs to* $\widetilde{\mathbf{\Lambda}} \times \mathbf{I}$ *be calculated and denoted by* $\mathcal{R}^{\Lambda}$. *Then, there exists a second-order tensor field* $\mathbf{r}^{\Lambda}$ *such that the following relations hold*

$$\mathbf{r}^{\Lambda}(\mathbf{u} \times \mathbf{v}) = (\mathcal{R}^{\Lambda}\mathbf{u})\mathbf{v} \quad \textit{and} \quad \mathbf{r}^{\Lambda} = \textit{curl}\ \widetilde{\mathbf{\Lambda}} + (\textit{Adj}\ \widetilde{\mathbf{\Lambda}})^T. \tag{24}$$

where $Adj(\widetilde{\mathbf{\Lambda}})$ *is defined by (4).*

Let C_0 be a closed curve (*a circuit*) in the reference configuration of the body and $\mathcal{A}_0$ be a surface with normal $\mathbf{N}$, which is surrounded by C_0.

The Frank vector is associated with a circuit C_0 and is viewed in the configuration with torsion, being defined by

$$\mathbf{\Omega}_{\mathcal{K}} = \int_{C_{\mathcal{K}}} \widetilde{\mathbf{\Lambda}}\ \mathrm{d}\mathbf{x}_{\mathcal{K}} = \int_{C_0} \widetilde{\mathbf{\Lambda}}\mathbf{F}^p\ \mathrm{d}\mathbf{X} = \int_{\mathcal{A}_0} \mathrm{curl}\left(\frac{1}{\det\mathbf{F}^p}\mathbf{F}^p\mathbf{\Lambda}\right)\mathbf{N}\mathrm{d}A \tag{25}$$

The disclination density with respect to the configuration with torsion is defined by

$$\boldsymbol{\alpha}^{\Lambda}_{\mathcal{K}} = \frac{1}{\det(\mathbf{F}^p)}\mathrm{curl}(\widetilde{\mathbf{\Lambda}}\mathbf{F}^p)(\mathbf{F}^p)^T, \tag{26}$$

as a consequence of the Frank vector formula (25) and the relationships between the corresponding surface measures in the reference configuration and in the configuration with torsion, namely

$$\mathbf{N}dA = \frac{1}{\det(\mathbf{F}^p)}\mathbf{F}^p\mathbf{n}_{\mathcal{K}}\mathrm{d}A_{\mathcal{K}}. \tag{27}$$

2.3 Measure of dislocations

The Burgers vector is defined in terms of the plastic distortion $\mathbf{F}^p$ and is associated with a circuit C_0 in the reference configuration, but it is viewed in the configuration with torsion (or the intermediate configuration). The Burgers vector associated with the circuit C_0 is defined by

$$\mathbf{b}_{\mathcal{K}} \equiv \left\{ \int_{C_{\mathcal{K}}} \mathrm{d}\mathbf{x}_{\mathcal{K}} \right\} = \int_{C_0} \mathbf{F}^p \, \mathrm{d}\mathbf{X} = \int_{\mathcal{A}_0} (\mathrm{curl}\mathbf{F}^p)\mathbf{N}\mathrm{d}A. \tag{28}$$

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

$$\boldsymbol{\alpha}_{\mathcal{K}} := \frac{1}{\det\mathbf{F}^p}(\mathrm{curl}\ \mathbf{F}^p)(\mathbf{F}^p)^T, \tag{29}$$

in configuration with torsion and it is called *Noll's dislocation density* or GND-dislocation density, being introduced by Noll [36].

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

Remark Le and Gunther [29] defined the true resultant Burgers vector according to $\mathbf{b} = (\mathbf{F}^p)^{-1}\int_{C_0} \mathbf{F}^p \, \mathrm{d}\mathbf{X}$ (in our notation). The authors mentioned that the value of $(\mathbf{F}^p)^{-1}$ can be taken at any point on the contour C_0; thus, we cannot say that the Burgers vector is dependent on the circuit only. From our point of view, a correct definition is given in (28) (following Teodosiu [42]), as the Burgers vector is associated with a curve and not with a material point.

2.4 Cartan torsion and defect densities

Starting from the definition of the Cartan torsion $\mathbf{S}^e_{\mathcal{K}}$ associated with the elastic connection derived in $(18)_2$, we prove the equalities

$$\begin{aligned} &((\mathbf{S}^e_{\mathcal{K}}\mathbf{u})\mathbf{v}) = \mathcal{N}^e_{\mathcal{K}}(\mathbf{u}\times\mathbf{v}),\\ &\mathcal{N}^e_{\mathcal{K}} = (\mathbf{F}^e)^{-1}\mathrm{curl}_{\mathcal{K}}\mathbf{F}^e - \left((\mathrm{tr}\ \widetilde{\boldsymbol{\Lambda}})\mathbf{I} - (\widetilde{\boldsymbol{\Lambda}})^T\right)\\ &\text{moreover}\quad (\mathbf{F}^e)^{-1}\mathrm{curl}_{\mathcal{K}}\mathbf{F}^e = \frac{1}{\det(\mathbf{F}^p)}(\mathrm{curl}\mathbf{F}^p)(\mathbf{F}^p)^T \equiv \boldsymbol{\alpha}_{\mathcal{K}}. \end{aligned} \tag{30}$$

$\mathbf{S}^e_{\mathcal{K}}$ defined in (30), via the second-order torsion tensor $\mathcal{N}^e_{\mathcal{K}}$, evokes the coupling between dislocations and disclinations continuously distributed.

Remark 2.1 $\mathrm{curl}_{\mathcal{K}}$ applied to $\mathbf{F}^e$ is taken in the configuration with torsion $\mathcal{K}$, and consequently, the basis vectors is $\mathbf{e}_j = \mathbf{F}^p\mathbf{G}_j$.

Remark 2.2 In the case of small plastic distortion,

$$\mathbf{F}^p = \mathbf{I} + \mathbf{H}^p, \quad \text{with} \quad |\ \mathbf{H}^p\ | \ll 1, \tag{31}$$

the *defect density tensors* are defined in terms of $\mathbf{H}^p$ and $\boldsymbol{\Lambda}$

$$\begin{aligned} &\boldsymbol{\alpha}_{\mathcal{K}} \simeq \mathrm{curl}\ \mathbf{F}^p, \quad \boldsymbol{\alpha}^{\boldsymbol{\Lambda}}_{\mathcal{K}} \simeq \mathrm{curl}(\widetilde{\boldsymbol{\Lambda}}), \quad \widetilde{\boldsymbol{\Lambda}} = \boldsymbol{\Lambda},\\ &\mathcal{N} \simeq \mathrm{curl}\ \mathbf{H}^p + (\mathrm{tr}\ \boldsymbol{\Lambda})\mathbf{I} - \boldsymbol{\Lambda}^T, . \end{aligned} \tag{32}$$

Remark 2.3 There exists a second-order tensor, $\boldsymbol{\kappa}^p$, which is incompatible and such that $\mathcal{N}$

$$\mathcal{N} = \text{curl}\, \boldsymbol{\varepsilon}^e + (\text{tr}\boldsymbol{\kappa}^p)\, \mathbf{I} - (\boldsymbol{\kappa}^p)^T, \qquad (33)$$
$$\boldsymbol{\kappa}^p = \boldsymbol{\Lambda} + \boldsymbol{\omega}^p.$$

Here, $\boldsymbol{\omega}^p$ is the vector coaxial with the skew-symmetric part of $\mathbf{H}^p$.

Consequently, under the supposition of small elasto-plastic distortions we proved the existence of $\boldsymbol{\kappa}^p$, which is an incompatible field, $\text{curl}\boldsymbol{\kappa}^p = \text{curl}\boldsymbol{\Lambda} \neq 0$. $\boldsymbol{\kappa}^p$ represents the so-called bent-twist or curvature tensor which is involved in the models proposed by de Wit [15–18], Fressengeas et al. [22] and Mayeur et al. [32].

3 Free energy imbalance principle formulated in $\mathcal{K}$

We introduce now the expression of the free energy density postulated with respect to the configuration with torsion. We assume that the free energy density is dependent on the second-order elastic deformation in terms of $(\mathbf{C}^e, \overset{(e)}{\mathcal{A}}_{\mathcal{K}})$, where $\mathbf{C}^e = (\mathbf{F}^e)^T\mathbf{F}^e$, and it is also influenced by the state of defects, i.e. $\mathbf{S}^e_{\mathcal{K}}$ and $\boldsymbol{\Lambda}$. The third-order torsion tensor $\mathbf{S}^e_{\mathcal{K}}$ is related to the elastic connection via the formula (30) and describes a coupling between the defects, and $\boldsymbol{\Lambda}$ is disclination tensor.

Ax.1: The *free energy density* is postulated to be dependent on the second-order elastic deformation, in terms of $(\mathbf{C}^e, \overset{(e)}{\mathcal{A}}_{\mathcal{K}})$, and on the defects through $(\mathbf{S}^e_{\mathcal{K}}, \widetilde{\boldsymbol{\Lambda}})$,

$$\psi = \psi_{\mathcal{K}}(\mathbf{C}^e, \overset{(e)}{\mathcal{A}}_{\mathcal{K}}, \mathbf{S}^e_{\mathcal{K}}, \widetilde{\boldsymbol{\Lambda}}), \quad \mathbf{C}^e = (\mathbf{F}^e)^T\mathbf{F}^e. \qquad (34)$$

Remark 3.1 The free energy density included the influence of the dislocation density $\boldsymbol{\alpha}_{\mathcal{K}}$ [see Definition (29) together with (30)] and disclination tensor $\widetilde{\boldsymbol{\Lambda}}$, both tensors being defined with respect to the configuration with torsion $\mathcal{K}$.

The elastic fields can be expressed through the second-order deformations associated with the motion and with the plastic behaviour, as a direct consequence of the relationships provided in Proposition 1, namely

$$\overset{(e)}{\mathcal{A}} = (\boldsymbol{\Gamma} - \overset{(p)}{\mathcal{A}})[(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}], \qquad (35)$$
$$\mathbf{C}^e = (\mathbf{F}^p)^{-T}\mathbf{C}(\mathbf{F}^p)^{-1}, \quad \mathbf{C} = \mathbf{F}^T\mathbf{F}.$$

3.1 Free energy imbalance principle

The local free energy imbalance principle states the internal power expended during the elasto-plastic process is equal or greater than the time derivative of the free energy density. The local free energy imbalance is formulated with respect to the configuration with torsion $\mathcal{K}$, since the defects are relevant at the level of the lattice microstructure.

Ax.2: The elasto-plastic constitutive description of the material is restricted to satisfy in $\mathcal{K}$ *the free energy imbalance principle*

$$(\mathcal{P}_{\text{int}})_{\mathcal{K}} - \dot{\psi}_{\mathcal{K}} \geq 0 \qquad (36)$$

for any virtual (isothermal) processes. Here, $(\mathcal{P}_{\text{int}})_{\mathcal{K}}$ denotes the internal power expanded during the elasto-plastic process in the configuration $\mathcal{K}$.

The free energy density function $\psi_{\mathcal{K}}$ is defined in (34).

We emphasize the set of independent kinematic variables, which are $\mathbf{L}, \mathbf{L}^p, \dot{\boldsymbol{\Lambda}}$ and their gradients. As a consequence of the multiplicative decomposition (8), the following kinematic relationships hold

$$\mathbf{L} = \mathbf{L}^e + \mathbf{F}^e\mathbf{L}^p(\mathbf{F}^e)^{-1}, \quad \mathbf{L}^e = \dot{\mathbf{F}}^e(\mathbf{F}^e)^{-1}, \quad \mathbf{L}^p = \dot{\mathbf{F}}^p(\mathbf{F}^p)^{-1}. \qquad (37)$$

Thus, the rate of elastic distortion $\mathbf{L}^e$ is dependent.

The expression of the internal power is the result of the superposed elastic, plastic and defect effects. We introduce the microstress and microstress momentum, namely $(\boldsymbol{\Upsilon}^p, \boldsymbol{\mu}_{\mathcal{K}})$, which are power conjugate with the rate of plastic distortion $\mathbf{L}^p$ and its gradient $\nabla_{\mathcal{K}}\mathbf{L}^p$ in the configuration with torsion. The microforces associated with the plastic behaviour are given by the microstress, $(\boldsymbol{\Upsilon}^p$, and microstress momentum, $\boldsymbol{\mu}^p$, and $\boldsymbol{\Upsilon}^\lambda$ is the microstress related to the disclination mechanism.

The microstress $\boldsymbol{\Upsilon}^\lambda$ is power conjugate with the rate of disclination tensor, $\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\boldsymbol{\Lambda}}$, and the influence of its gradient is not considered.

The macroforces, the non-symmetric Cauchy stress $\mathbf{T}$ and macrostress momentum $\boldsymbol{\mu}_{\mathcal{K}}$, are power conjugate with the rate of elastic distortion, $\mathbf{L}^e$, and an appropriate measure of its gradient, the so-called *second-order elastic distortion rate* which is expressed by

$$(\mathcal{L}_{\mathbf{L}^p}[\overset{(e)}{\mathcal{A}}_{\mathcal{K}}]) = (\mathbf{F}^e)^{-1}(\nabla_\chi \mathbf{L})[\mathbf{F}^e, \mathbf{F}^e] - \nabla_{\mathcal{K}}\mathbf{L}^p. \tag{38}$$

Remark 3.2 The expression written in the right-hand side of (38) represents the difference between the second-order velocity gradient, which is pulled back to the configuration $\mathcal{K}$, and the gradient of the plastic distortion rate again written with respect to $\mathcal{K}$.

$(\mathcal{P}_{\text{int}})_{\mathcal{K}}$ will be written here in a slightly modified version of the corresponding expression in [11].

Ax.3: The internal power in the *configuration with torsion* is postulated to be given by the expression

$$\begin{aligned}(\mathcal{P}_{\text{int}})_{\mathcal{K}} = \frac{1}{\rho}(\mathbf{T}^s)\cdot\mathbf{L}^e + \frac{1}{\widetilde{\rho}}\boldsymbol{\Upsilon}^p\cdot\mathbf{L}^p + \frac{1}{\widetilde{\rho}}\boldsymbol{\mu}^p\cdot\nabla_{\mathcal{K}}\mathbf{L}^p \\ + \frac{1}{\widetilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}}\cdot(\mathcal{L}_{\mathbf{L}^p}[\overset{(e)}{\mathcal{A}}_{\mathcal{K}}]) + \frac{1}{\widetilde{\rho}}\boldsymbol{\Upsilon}^\lambda\cdot\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\boldsymbol{\Lambda}}.\end{aligned} \tag{39}$$

Here, ∇_χ denotes the gradient with respect to the deformed configuration of the body $\mathcal{B}$.

In order to investigate the consequences derived from the free energy imbalance principle (36), we follow the steps:

1. The time derivative of the free energy is computed by

$$\dot{\psi} = \partial_{\mathbf{C}^e}\psi\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{C}^e) + \partial_{\mathcal{A}}\psi\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\overset{(e)}{\mathcal{A}}_{\mathcal{K}}) + \partial_{\mathbf{S}}\psi\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{S}^e_{\mathcal{K}}) + \partial_{\widetilde{\boldsymbol{\Lambda}}}\psi\cdot\frac{\mathrm{d}}{\mathrm{d}t}(\widetilde{\boldsymbol{\Lambda}}), \tag{40}$$

   and the derivatives of the mentioned fields will be replaced by their appropriate expressions;
2. Under the supposition that no evolution of the plastic distortion and disclination mechanism occurs (which means that $\mathbf{L}^p = 0$ and $\dot{\widetilde{\boldsymbol{\Lambda}}} = 0$), the elastic-type constitutive equations for macroforces are derived;
3. The reduced dissipation inequality is emphasized;
4. The possible consequences that follow from the reduced dissipation inequality can be derived to express the evolutions of plastic distortion and disclination tensor.

In (40), the rates of the considered fields are replaced by their appropriate expressions.

The time derivative of the formula $(13)_2$ is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}(\overset{(e)}{\mathcal{A}}_{\mathcal{K}}) = (\mathcal{L}_{\mathbf{L}^p}[\overset{(e)}{\mathcal{A}}_{\mathcal{K}}]) + \mathbf{L}^p\,\overset{(e)}{\mathcal{A}}_{\mathcal{K}} - \overset{(e)}{\mathcal{A}}_{\mathcal{K}}\,\mathbf{L}^p - \overset{(e)}{\mathcal{A}}_{\mathcal{K}}\,[\mathbf{I}, \mathbf{L}^p], \tag{41}$$

together with (38). The formula $(30)_1$ leads to

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{S}^e_{\mathcal{K}}) = Skw\left\{\frac{\mathrm{d}}{\mathrm{d}t}(\overset{(e)}{\mathcal{A}}_{\mathcal{K}})\right\} - Skw\left\{\left(\frac{\mathrm{d}}{\mathrm{d}t}\widetilde{\boldsymbol{\Lambda}}\right)\times\mathbf{I}\right\}. \tag{42}$$

As a consequence of the formula $(34)_2$ together with (37) the formula

$$\dot{\mathbf{C}}^e = 2(\mathbf{F}^e)^T\mathbf{D}^e\mathbf{F}^e, \quad \mathbf{D}^e = \{\mathbf{L}^e\}^s. \tag{43}$$

follows.

Proposition 3.1 *The free energy imbalance principle (36) is reformulated as the inequality written below*

$$\begin{aligned}
&\left\{\frac{1}{\rho}\{\mathbf{T}\}^S - 2\mathbf{F}^e\partial_{\mathbf{C}^e}\psi(\mathbf{F}^e)^T\right\}\cdot\ \mathbf{L}^e + \frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^p\cdot\mathbf{L}^p + \frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p\cdot\nabla_{\mathcal{K}}\mathbf{L}^p\\
&+\left(\frac{1}{\tilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}} - (\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)\right)\cdot((\mathbf{F}^e)^{-1}(\nabla_\chi\mathbf{L})[\mathbf{F}^e,\mathbf{F}^e] - \nabla_{\mathcal{K}}\mathbf{L}^p)\\
&-(\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)\cdot\left(\mathbf{L}^p\overset{(e)}{\mathcal{A}_{\mathcal{K}}} - \overset{(e)}{\mathcal{A}_{\mathcal{K}}}\mathbf{L}^p - \overset{(e)}{\mathcal{A}_{\mathcal{K}}}[\mathbf{I},\mathbf{L}^p]\right)\\
&+\left(\frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^\lambda - \partial_{\tilde{\boldsymbol{\Lambda}}}\psi\right)\cdot\dot{\tilde{\boldsymbol{\Lambda}}} + \partial_{\mathbf{S}^e}\psi\cdot(Skw\{\dot{\tilde{\boldsymbol{\Lambda}}}\times\mathbf{I}\}) \geq 0.
\end{aligned}\tag{44}$$

If we suppose that no evolution of the plastic distortion and of the disclination mechanism occurs, which means that $\mathbf{L}^p = 0$ and $\dot{\tilde{\boldsymbol{\Lambda}}} = 0$, then $\mathbf{L}^e = \mathbf{L}$, and from (41) together with (38), we get

$$\frac{\mathrm{d}}{\mathrm{d}t}(\overset{(e)}{\mathcal{A}_{\mathcal{K}}}) = (\mathcal{L}_{\mathbf{L}^p}[\overset{(e)}{\mathcal{A}_{\mathcal{K}}}]) = (\mathbf{F}^e)^{-1}(\nabla_\chi\mathbf{L})[\mathbf{F}^e,\mathbf{F}^e].\tag{45}$$

Consequently, the free energy imbalance is rewritten as

$$\begin{aligned}
&\left\{\frac{1}{\rho}\{\mathbf{T}\}^S - 2\mathbf{F}^e\partial_{\mathbf{C}^e}\psi(\mathbf{F}^e)^T\right\}\cdot\ \mathbf{L}\\
&+\left(\frac{1}{\tilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}} - \partial_{\mathcal{A}^e}\psi - \partial_{\mathbf{S}^e}\psi\right)\cdot(\mathbf{F}^e)^{-1}(\nabla_\chi\mathbf{L})[\mathbf{F}^e,\mathbf{F}^e] \geq 0
\end{aligned}\tag{46}$$

for any virtual process, i.e. $\forall\ \mathbf{L}$, $\nabla_\chi\mathbf{L}$.

Theorem 3.1 *1. The thermomechanics restrictions imposed to the elastic-type constitutive functions are*

$$\begin{aligned}
&\frac{1}{\rho}\{\mathbf{T}\}^s = 2\mathbf{F}^e(\partial_{\mathbf{C}^e}\psi)(\mathbf{F}^e)^T,\\
&\frac{1}{\tilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}} = \partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi.
\end{aligned}\tag{47}$$

2. The reduced dissipative inequality has to be satisfied

$$\begin{aligned}
&\frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^p\cdot\mathbf{L}^p + \frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p\cdot\nabla_{\mathcal{K}}\mathbf{L}^p + \{(\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)_r\odot\overset{(e)}{\mathcal{A}_{\mathcal{K}}}\\
&-(\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)\odot_l\overset{(e)}{\mathcal{A}_{\mathcal{K}}} - (\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)\odot\overset{(e)}{\mathcal{A}_{\mathcal{K}}}\}\cdot\mathbf{L}^p\\
&+\left(\frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^\lambda - \partial_{\tilde{\boldsymbol{\Lambda}}}\psi\right)\cdot\dot{\tilde{\boldsymbol{\Lambda}}} + \partial_{\mathbf{S}^e}\psi\cdot(Skw\{\dot{\tilde{\boldsymbol{\Lambda}}}\times\mathbf{I}\}) \geq 0.
\end{aligned}\tag{48}$$

Proposition 3.2 *The following formula can be derived taking into account the formula (5)*

$$\partial_{\mathbf{S}^e}\psi\cdot(Skw\{\dot{\tilde{\boldsymbol{\Lambda}}}\times\mathbf{I}\}) = -(\in\odot_l\ \partial_{\mathbf{S}^e}\psi)\cdot\dot{\tilde{\boldsymbol{\Lambda}}},\tag{49}$$

by considering that "∈" denotes Ricci's permutation symbol.

3.2 Viscoplastic-type constitutive equations for microforces

Based on the reduced dissipation inequality written in (48), we formulate the *constitutive hypotheses* in plastically deformed configuration:

Ax.5 The microforces contain:

(1) a *dissipative part*, and
(2) a non-dissipative part, which is derived from the free energy, the so-called *energetic microforces*.

The plastic microstress is represented through the coupled relationship

$$\frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^p + (\partial_{\mathcal{A}}\psi + \partial_{\mathbf{S}^e}\psi)_r \odot \overset{(e)}{\mathcal{A}_{\mathcal{K}}} - (\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)\odot_l \overset{(e)}{\mathcal{A}_{\mathcal{K}}} - (\partial_{\mathcal{A}^e}\psi + \partial_{\mathbf{S}^e}\psi)\odot \overset{(e)}{\mathcal{A}_{\mathcal{K}}} = \xi_1\, \mathbf{L}^p, \tag{50}$$

and the microstress associated with disclinations is characterized by

$$\frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^\lambda - \partial_{\tilde{\boldsymbol{\Lambda}}}\ \psi - (\in \odot_l\ \partial_{\mathbf{S}^e}\psi) = \xi_2\ \dot{\tilde{\boldsymbol{\Lambda}}}. \tag{51}$$

$\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p = 0$, i.e. the micromomentum related to the plastic behaviour is vanishing, i.e.

Ax.6 The scalar constitutive functions ξ_1 and ξ_2 are defined in such a way to be compatible with the dissipation inequality

$$\xi_1\ \mathbf{L}^p \cdot \mathbf{L}^p + \xi_2 \dot{\tilde{\boldsymbol{\Lambda}}} \cdot \dot{\tilde{\boldsymbol{\Lambda}}} \geq 0. \tag{52}$$

Remark 3.3 The constitutive functions ξ_1 and ξ_2, which are involved in (50) and (51), can be determined to be compatible with the reduced dissipation inequality (52), following the similar procedures to those developed for instance in [9] and [12].

Ax.7 As the micromomentum related to plastic mechanism is not involved in the internal dissipated power, the microforce $\boldsymbol{\Upsilon}^p$ can be identified with the Mandel stress measure, which is power conjugated with the plastic distortion rate $\mathbf{L}^p$, namely

$$\frac{1}{\tilde{\rho}}\boldsymbol{\Upsilon}^p = \frac{1}{\tilde{\rho}}\boldsymbol{\Sigma}^p = \frac{1}{\rho}(\mathbf{F}^e)^T\{\mathbf{T}\}^S(\mathbf{F}^e)^{-T}. \tag{53}$$

3.3 Conclusions

Here, we developed the constitutive framework for elasto-plastic solids with structural defects, like dislocations and disclinations. The incompatibility tensors, namely the so-called defect density tensors, have been considered to be basic kinematic fields which are involved in the material description. The behaviour of the model is described with respect to the so-called configuration with torsion. $\mathbf{S}^e_{\mathcal{K}}$ characterizes the cumulative effect of dislocation and disclination, while $\tilde{\boldsymbol{\Lambda}}$ is a measure of disclination at the level of the crystalline lattice.

The viscoplastic-type constitutive equations which describe the evolution of plastic distortion and disclination tensor are derived to be compatible with the free energy imbalance principle. As the microstress associated with the disclination mechanism remains undefined in the model performed here, $\tilde{\boldsymbol{\Lambda}}$ can be viewed as internal variable, see for instance the discussion concerning this issue in [31]. Consequently, it is possible to take

$$\boldsymbol{\Upsilon}^\lambda = \tilde{\rho}\partial_{\tilde{\boldsymbol{\Lambda}}}\ \psi \tag{54}$$

The various models with defects can be derived within the constitutive framework described here, which correspond to the possible expressions for the free energy function given with respect to the configuration with torsion. For instance, the following *hypothesis* can be considered: the *free energy density* is a quadratic function with respect to the second-order elastic deformation, written in terms of $(\mathbf{C}^e, \overset{(e)}{\mathcal{A}}_{\mathcal{K}})$, and to a measure of defects represented by $(\mathbf{S}^e_{\mathcal{K}}, \widetilde{\boldsymbol{\Lambda}})$. Let us consider the free energy density given by

$$\psi = \mathcal{E}\frac{1}{2}(\mathbf{C}^e - \mathbf{I})\cdot(\mathbf{C}^e - \mathbf{I}) + \frac{1}{2}\beta_1 \overset{(e)}{\mathcal{A}}_{\mathcal{K}} \cdot \overset{(e)}{\mathcal{A}}_{\mathcal{K}} + \frac{1}{2}\beta_2 \mathbf{S}^e_{\mathcal{K}} \cdot \mathbf{S}^e_{\mathcal{K}} + \frac{1}{2}\beta_3 \widetilde{\boldsymbol{\Lambda}} \cdot \widetilde{\boldsymbol{\Lambda}}. \tag{55}$$

To describe the behaviour of elasto-plastic materials with structural defects, such as dislocation and disclination, the initial and boundary value problems have to be formulated within the constitutive framework considered here.

- The local balance law for linear momentum equation to be satisfied by the non-symmetric Cauchy stress, $\mathbf{T}$, and the macrostress momentum $\boldsymbol{\mu}$ (which is described as a third-order tensor) was written in (1), in the deformed configuration of the body.
- The constitutive equation for macroforces are written in (47) in terms of the symmetric part of Cauchy stress, $\mathbf{T}$, and macrostress momentum in $\mathcal{K}$, $\boldsymbol{\mu}_{\mathcal{K}}$. The macromomentum in the deformed configuration, $\boldsymbol{\mu}$, represents the pushed away momentum from the configuration with torsion $\mathcal{K}$, being related by

$$\frac{\boldsymbol{\mu}}{\rho} = (\mathbf{F}^e)^{-T}\frac{\boldsymbol{\mu}_{\mathcal{K}}}{\tilde{\rho}}[(\mathbf{F}^e)^T, (\mathbf{F}^p)^T]. \tag{56}$$

- The evolution equation for plastic distortion is given by (50) together with (53)

$$\begin{aligned}\xi_1\, \mathbf{L}^p = \frac{1}{\rho}(\mathbf{F}^e)^T\{\mathbf{T}\}^S(\mathbf{F}^e)^{-T} + (\partial_{\mathcal{A}}\psi + \partial_{\mathbf{S}^e}\psi)_r \odot \overset{(e)}{\mathcal{A}}_{\mathcal{K}} \\ - (\partial_{\mathcal{A}}\psi + \partial_{\mathbf{S}^e}\psi)\odot_l \overset{(e)}{\mathcal{A}}_{\mathcal{K}} - (\partial_{\mathcal{A}}\psi + \partial_{\mathbf{S}^e}\psi)\odot \overset{(e)}{\mathcal{A}}_{\mathcal{K}}\,.\end{aligned} \tag{57}$$

- The evolution in time of the disclination tensor is described by (51) together with (54)

$$\xi_2\, \dot{\widetilde{\boldsymbol{\Lambda}}} = -(\in \odot_l\ \partial_{\mathbf{S}^e}\psi). \tag{58}$$

The expression of the free energy density (55) can be rewritten with third-order tensorial fields replaced by the appropriate second-order tensors, using the procedure provided in [9].

The models performed here avoids the singularities existing along the dislocation and disclination lines in the elastic models.

Acknowledgments This work was supported by the Romanian National Authority for Scientific Research (CNCS-UEFISCDI; project number PN II-ID-PCE-2011-3-0521). The very constructive comments and suggestions made by the anonymous reviewers are gratefully acknowledged.

References

1. Acharya, A., Bassani, J.L.: Lattice incompatibility and gradient theory of crystal plasticity. J. Mech. Phys. Solids **48**, 1565–1595 (2000)
2. Arsenlis, A., Parks, D.M.: Crystallographic aspects of geometrically-necessary and statistically-stored dislocation density. Acta Mater. **47**, 1597–1611 (1999)
3. Bilby, B.A.: Continuous distribution of dislocations. In: Sneddon, I.N., Hill, R. (eds.) Progress in Solid Mechanics, pp. 329–398. North-Holland, Amsterdam (1960)
4. Cermelli, P., Gurtin, M.E.: On the characterization of geometrically necessary dislocations in finite plasticity. J. Mech. Phys. Solids **48**, 1539–1568 (2001)
5. Clayton, J.D., McDowell, D.L., Bammann, D.J.: Modeling dislocations and disclinations with finite micropolar elastoplasticity. Int. J. Plast. **22**, 210–256 (2006)
6. Clayton, J.D., Bammann, D.J., McDowell, D.L.: Anholonomic configuration spaces and metric tensors in finite elastoplasticity. Int. J. Non-linear Mech. **39**:1039–1049 (2004)
7. Clayton, J.D.: On anholonomic deformation, geometry, and differentiation. Math. Mech. Solids **17**, 702–735 (2012)
8. Cleja-Ţigoiu, S., Soós, E.: Elastoplastic models with relaxed configurations and internal state variables. Appl. Mech. Rev. **43**, 131–151 (1990)
9. Cleja-Ţigoiu, S., Ţigoiu, V.: Strain gradient Effects in Finite Elasto-plastic Damaged Materials. Int. J. Damage Mech. **20**, 484–577 (2011)
10. Cleja-Ţigoiu, S.: Material forces in finite elasto-plasticity with continuously distributed dislocations. Int. J. Fract. **147**, 67–81 (2007)

11. Cleja-Ţigoiu, S.: Elasto-plastic materials with lattice defects modeled by second order deformations with non-zero curvature. Int. J. Fract. **166**, 61–75 (2010)
12. Cleja-Ţigoiu, S.: Non-local elasto-viscoplastic models with dislocations in finite elasto-plasticity. Part I: Constitutive framework. Math. Mech. Solids **18**(4), 349–372 (2013)
13. Cross, J.J.: Mixture of fluids and isotropic solids. Arch. Mech. **25**(6), 1025–1039
14. Deng, S., Liu, J., Liang, N.: Wedge and twist disclinations in second strain gradient elasticity. Int. J. Solids Struct. **44**, 3646–3665 (2007)
15. de Wit, R.: Linear theory of static disclinations. In: Simmons, J.A., de Wit, R., Bullough, R. (eds.) Fundamental Aspects of Dislocation Theory, vol. 317, I, pp. 651–673. Nat. Bur. Stand. (US), Spec. Publ. (1970)
16. de Wit, R.: Theory of disclinations: II. Continuous and discrete disclinations in anisotropic elasticity. J. Res. Natl. Bureau Stand. A Phys. Chem. **77**(1), 49–100 (1973)
17. de Wit, R.: Theory of disclinations: III. Continuous and discrete disclinations in isotropic elasticity. J. Res. Natl. Bureau Stand. A Phys. Chem. **77**(3), 359–368 (1973)
18. de Wit, R.: Theory of disclinations: IV. Straight disclinations. J. Res. Natl. Bureau Stand. A. Phys. Chem. **77**(5), 607–658 (1973)
19. R. de Wit, A view of the relation between the continuum theory of lattice defects and non-Euclidean geometry in the linear approximation. Int. J. Eng. Sci. **19**, 1475–1506 (1981)
20. Epstein, M., Maugin, G.A.: The energy-momentum tensor and material uniformity in finite elasticity. Acta Mecanica **83**, 127–133 (1990)
21. Fleck, N.A., Muller, G.M., Ashby, M.F., Hutchinson, J.W.: Strain gradient plasticity: theory and experiment. Acta Metall. Mater. **42**, 475–487 (1994)
22. Fressengeas, C., Taupin, V., Capolungo, L.: An elasto-plastic theory of dislocation and disclination field. Int. J. Solids Struct. **48**, 3499–3509 (2011)
23. Gurtin, M.E., Fried, E., Anand, L.: The Mechanics and Thermodynamics of Continua. University Press, Cambridge (2010)
24. Gutkin, M., Aifantis, E.C.: Dislocations and disclinations in gradient theory of elasticity. Phys. Solid State **41**(12), 1980–1988 (1999)
25. Kossecka, E., de Wit, R.: Disclination kinematics. Arch. Mech. **29**(5), 633–650 (1977)
26. Kröner, E.: The differential geometry of elementary point and line defects in Bravais crystals. Int. J. Theor. Phys. **29**, 1219–1237 (1990)
27. Kröner, E.: The internal mechanical state of solids with defects. Int. J. Solids Struct. **29**, 1849–1857 (1992)
28. Lazar, M., Maugin, G.A., Aifantis, E.C.: Nonsingular stress and strain fields of dislocations and disclinations in first strain gradient elasticity. Int. J. Solids Struct. **43**, 1787–1817 (2006)
29. Le, K.C., Günther, C.: Nonlinear continuum dislocation theory revisited. Int. J. Plast. **53**, 164–178 (2014)
30. Mandel, J.: Plasticité classique et viscoplasticité, CISM- Udine. Springer, Vienna (1972)
31. Maugin, G.A.: Internal variables and dissipative structures. J. Non-Equilib. Thermodyn. **15**, 173–192 (1990)
32. Mayeur, J.R., McDowell, D.L., Bammann, D.J.: Dislocation-based micropolar single crystal plasticity: Comparison of multi-and single criterion theories. J. Mech. Phys. Solids **59**, 398–422 (2011)
33. Mayeur, J.R., McDowell, D.L.: Bending of single crystal thin films modeled with micropolar crystal plasticity. Int. J. Eng. Sci. **49**, 1357–1366 (2011)
34. Mecking, H., Kocks, U.F.: Kinetics of flow and strain-hardening. Acta Metall. **29**, 1865–1875 (1981)
35. Mura, T.: Micromechanics of Defects in Solids. Martinus Nijhoff Publishers, Boston (1982)
36. Noll, W.: Materially Uniform Simple Bodies with Inhomogeneities. Arch. Rat. Mech. Anal. 1967, and in The Foundations of Mechanics and Thermodynamics, Selected papers. Springer, Berlin (1974)
37. Romanov, A.E.: Mechanics and physics of disclinations in solids. Eur. J. Mech. A/Solids **22**, 727–741 (2003)
38. Romanov, A.E., Kolesnikova, A.L.: Application of disclination concept to solid structures. Prog. Mater. Sci. **54**, 740–769 (2009)
39. Schouten, J.A.: Ricci-Calculus. Springer, Heidelberg (1954)
40. Seefeldt, M., Klimanek, P.: Modelling of flow behaviour of metals by means of a dislocation-disclination reaction kinetics. Model. Simul. Mater. Sci. Eng. **6**, 349–360 (1998)
41. Seefeldt, M., Klimanek, P.: Interpretation of plastic deformation by means of dislocation-disclination reaction kinetics. Mater. Sci. Eng. **A234-236**, 758–761 (1997)
42. Teodosiu, C.: A dynamic theory of dislocations and its applications to the theory of the elastic-plastic continuum. In: Simmons, J.A., de Witt, R., Bullough, R. (eds.) Fundamental Aspects of Dislocation Theory, vol. 317, II, pp. 837– 876. Nat. Bur. Stand. (US), Spec. Publ. (1970)
43. Teodosiu, C.: Elastic Models of Crystal Defects. Ed. Academiei. Springer, Berlin (1982)
44. Walgraef, D., Aifantis, D.E.C.: Plastic instabilities, dislocation patterns and nonequilibrium phenomena. Res. Mech. **23**, 161–195 (1988)
45. Walgraef, D., Aifantis, D.E.C.: Dislocation inhomogeneity in cyclic deformation. In: Weng, G.J., Taya, M., Abe, H. (eds.) Micromechanics and Inhomogeneity: The Toshio Mura Anniversary Volume, pp. 511–533. Spinger, Berlin (1990)
46. Wang, C.C.: Inhomogeneities in second-grade fluid bodies and isotropic solid bodies. Arch. Mech. **25**, 765–780 (1973)
47. Yavari, A.: Riemann–Cartan geometry of nonlinear dislocation mechanics. Arch. Ration. Mech. Anal. **205**, 59–118 (2012)