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DISLOCATIONS AND DISCLINATIONS IN FINITE ELASTO-PLASTICITY

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Abstract The paper deals with analytical description of the dislocation and disclination, which are lattice defects of the crystalline materials. The evolution equations for disclinations, having as source the screw dislocations are derived within the constitutive framework of second order plasticity developed by the author in the papers appeared in Int. J. Fracture (2007), (2010).

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1. INTRODUCTION

The plastic deformability of metals, which are crystalline materials, is produced because of the existence of lattice defects inside the microstructure. The lattice defects, among which the dislocations, disclinations and point defects are mathematically modeled by the differential geometry concepts, as torsion, curvature and metric property of certain connection, see Kröner [10], [11], de Wit [7], but without any elasto-plastic constitutive equations. The elastic models for crystal defects can be found in Teodosiu [14]. We are not dealing *with curved space* but *with curved geometry in flat space* as stated de Wit [7].

1. The nature of the geometry is determined by the *linear connection* $\mathbf{\Gamma}$, fixed by its coefficients, *the curvature tensor* $\mathcal{R}$, *the Cartan torsion* or *torsion tensor* $\mathbf{S}$;

2. *the metric tensor* $\mathbf{C}$, to measure the distance;

3. *the non-metricity measure* $\mathbf{Q}$, of the connection relative to the metric tensor, i.e. in terms of $\mathbf{\Gamma}$ and $\mathbf{C}$.

Geometry for which $\mathcal{R}, \mathbf{S}, \mathbf{Q}$ are non-vanishing is *non-metric, non-Riemannian*. We restrict ourself to the case $\mathbf{Q} = 0$, which means that the geometry is *metric*. If $\mathcal{R} = 0$ the geometry is called *flat*. If $\mathbf{S} = 0$ the geometry is called *symmetric*. If $\mathbf{S} = 0$ the geometry is called *Riemannian*. If $\mathcal{R} = 0, \mathbf{S} = 0$ geometry is called *Euclidean*.

In this paper the dislocations and disclinations are lattice defects of interest. The *dislocations* are characterized by *the Cartan torsion*, or by the non-zero *curl* of plastic connection, which means that the plastic distorsion can not be derived from a certain potential. The *disclinations* are characterized by a *non-vanishing curvature* $\mathcal{R}$.

The mathematical description of the continuously distributed dislocations is given by Noll [13], and the differential geometry support within the context of continuum mechanics can be found also in [12].

In this paper a peculiar mathematical problem is analyzed: find the disclinations, which are solutions of the appropriate evolution equation in such a way that the micro balance equation are satisfied, when the distribution of the dislocations is given.

To give the mathematical description of the problem, we precise the general constitutive framework which is able to capture the dislocations and disclinations. We mention here the direction developed by Clayton et al. [3] within a micropolar elasto-plastic model, in order to emphasize the *translational* (dislocation) and *rotational* (disclinaton) defects.

The behaviour of elasto-plastic body is described within the constitutive framework of second order plasticity, see Cleja-Ţigoiu [5], [6], based on the decomposition rule of the motion connection into the elastic and plastic second order deformations, see Cleja-Ţigoiu [4], and on the *existence of configurations with torsion*. The so called configuration with torsion is denoted by $\mathcal{K}$, and it is described through a pair, composed by $\mathbf{F}^p$, an invertible second order tensor which is called *plastic distorsion* and $\overset{(p)}{\mathbf{\Gamma}}$, a third order tensor field which is called *plastic connection*.

The pair $(\mathbf{F}^p, \overset{(p)}{\mathbf{\Gamma}})$ defines the *second order plastic deformation* with respect to the reference configuration of the body $\mathcal{B}$. The actual configuration of the body is associated with t he motion function, which is defined at every time t by $\chi(\cdot, t) : \mathcal{B} \longrightarrow \mathcal{E}$, $\mathcal{E}$ being the Euclidean (flat space) with a three dimensional vector space $\mathcal{V}$. The second order elastic deformation, as a consequence of the decomposition rule, is defined with respect to the so called configuration with torsion $\mathcal{K}$, which is time dependent. Two type of forces, macro and micro forces, are considered in the model. They are viewed as pairs of *stress* (a second order tensorial field) and *stress momentum* (a third order tensorial field), and they obey their own balance laws. The micro forces satisfy the viscoplastic type constitutive equations, in $\mathcal{K}_t$. The evolution equations for $\mathcal{K}_t$, which means the plastic distortion and plastic connection, have to be given. They have been derived to be compatible with an appropriate dissipation postulate. The *energetic arguments*, like a *virtual power principle*, *macro and micro balance equations*, and especially a dissipation postulate (see energy imbalance principle, for instance in Gurtin [9]) in order to prove *thermomechanics restrictions*, see Gurtin [9], Cleja-Ţigoiu [5].

In our adopted formalism the measure of the dislocations is characterized by the non-vanishing plastic curl (see Bilby [1], Noll [13]), while the disclinations has been related to a certain second order tensor $\mathbf{\Lambda}$ which enters the expression of the plastic connection and generates a non-zero curvature, apart from de Wit [7], where a measure of disclination is considered to be a second order curvature tensor.

The following notations, definitions and relationships will be used in the paper:

$\mathbf{u}\cdot\mathbf{v}, \mathbf{u}\times\mathbf{v}, \mathbf{u}\otimes\mathbf{v}$ denote scalar, cross and tensorial products of vectors;
$\mathbf{a}\otimes\mathbf{b}$ and $\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c}$ are a second order tensor and a third order tensor defined by $(\mathbf{a}\otimes\mathbf{b})\mathbf{u} = \mathbf{a}(\mathbf{b}\cdot\mathbf{u})$, $\quad(\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c})\mathbf{u} = (\mathbf{a}\otimes\mathbf{b})(\mathbf{c}\cdot\mathbf{u})$, for all vectors $\mathbf{u}$.
For $\mathbf{A}\in Lin$ (*Lin*- the space of second order tensors), we introduce:
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*, $\mathbf{A}^T$ denotes the transpose of $\mathbf{A}\in Lin$,
$\nabla\mathbf{A}$ is the derivative (or the gradient) of the field $\mathbf{A}$ in a coordinate system $\{\mathbf{x}^a\}$ (with respect to the reference configuration), $\nabla\mathbf{A} = \dfrac{\partial A_{ij}}{\partial x^k}\mathbf{e}^i\otimes\mathbf{e}^j\otimes\mathbf{e}^k$.

Definition 1.1. *The curl operator is defined for any smooth second order field, say* $\mathbf{A}$*, through*

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

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

The scalar product of two second order tensor $\mathbf{A},\mathbf{B}$ is $\mathbf{A}\cdot\mathbf{B} := \mathrm{tr}(\mathbf{A}\mathbf{B}^T) = A_{ij}B_{ij}$, and the scalar product of third order tensors is given by $\mathbf{N}\cdot\mathbf{M} = N_{ijk}M_{ijk}$, in a Cartesian coordinate system. $\mathbf{AB}$ denotes the composition of $\mathbf{A},\mathbf{B}\in Lin$. The compositions of $\mathbf{A}\in Lin$ and $\mathcal{N}$, a third order tensor, defines the appropriate third order tensorial fields, via the formulae $\mathcal{N}\mathbf{A}\mathbf{u} = \mathcal{N}_{ijk}\mathbf{A}_{kp}u_p\mathbf{i}^i\otimes\mathbf{i}^j$, and $\mathbf{A}\mathcal{N}\mathbf{u} = A_{ij}\mathcal{N}_{jpk}u_k\mathbf{i}^i\otimes\mathbf{i}^p$, which are written in a Cartesian basis, for any vector $\mathbf{u}$.

The affine connection is defined in a coordinate system by its coordinate representation

$$\mathbf{\Gamma} = \Gamma^i_{mk}\mathbf{e}_i\otimes\mathbf{e}^m\otimes\mathbf{e}^k. \tag{2}$$

We introduce the third order tensor field $\mathbf{\Gamma}[\mathbf{F}_1,\mathbf{F}_2]$, which is generated by a third order field $\mathbf{\Gamma}$ together with the second order tensors $\mathbf{F}_1,\mathbf{F}_2$ through the formula

$$(\mathbf{\Gamma}[\mathbf{F}_1,\mathbf{F}_2]\mathbf{u})\mathbf{v} = (\mathbf{\Gamma}(\mathbf{F}_1\mathbf{u}))\,\mathbf{F}_2\mathbf{v}, \quad \forall\mathbf{u},\mathbf{v}\in\mathcal{V}. \tag{3}$$

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

$$((\mathbf{\Lambda}_1\times\mathbf{\Lambda}_2)\mathbf{u})\mathbf{v} = (\mathbf{\Lambda}_1\mathbf{u})\times(\mathbf{\Lambda}_2\mathbf{v}), \quad \forall\mathbf{u},\mathbf{v}\in\mathcal{V}. \tag{4}$$

For $\mathcal{A}$, a third order tensor, we define the vector field $\mathrm{tr}_{(2)}\mathcal{A}$ through the relationship written for all vectors

$$(\mathrm{tr}_{(2)}\mathcal{A})\cdot\mathbf{u} = \mathrm{tr}(\mathcal{A}\mathbf{u}). \tag{5}$$

Three types of second order tensors, $\mathcal{A}\odot\mathcal{B}$, $\mathcal{A}\,{}_r\!\odot\mathcal{B}$ and $\mathcal{A}\odot_l\mathcal{B}$ will be associated with any pair $\mathcal{A},\mathcal{B}$ of third order tensors, following the rules written for all $\mathbf{L}\in Lin$

$$\begin{aligned}
(\mathcal{A}\odot\mathcal{B})\cdot\mathbf{L} &= \mathcal{A}[\mathbf{I},\mathbf{L}]\cdot\mathcal{B} = \mathcal{A}_{isk}L_{sn}\mathcal{B}_{ink}\\
(\mathcal{A}\,{}_r\!\odot\mathcal{B})\cdot\mathbf{L} &= \mathcal{A}\cdot(\mathbf{L}\mathcal{B}) = \mathcal{A}_{ijk}L_{in}\mathcal{B}_{njk}\\
(\mathcal{A}\odot_l\mathcal{B})\cdot\mathbf{L} &= \mathcal{A}\cdot(\mathcal{B}\mathbf{L}) = \mathcal{A}_{ijk}\mathcal{B}_{ijn}L_{kn}.
\end{aligned} \tag{6}$$

2. GEOMETRIC RELATIONSHIPS

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

$\nabla_\chi\mathbf{F}$ is a gradient in the actual configuration, while the gradient in the configuration with torsion $\mathcal{K}$, $\nabla_\mathcal{K}\mathbf{F}$, is calculated by

$$\nabla_\mathcal{K}\mathbf{F} := (\nabla\mathbf{F})(\mathbf{F}^p)^{-1}. \tag{7}$$

Ax.1 The decomposition of the second order deformation, $(\mathbf{F}, \mathbf{\Gamma})$, associated with the motion of the body $\mathcal{B}$, into elastic, $(\mathbf{F}^e, \overset{(e)}{\mathbf{\Gamma}}_\mathcal{K})$, and plastic, $(\mathbf{F}^p, \overset{(p)}{\mathbf{\Gamma}})$, second order deformations is given by

$$\begin{aligned} &\mathbf{F} = \mathbf{F}^e\mathbf{F}^p, \\ &\mathbf{\Gamma} = \overset{(p)}{\mathbf{\Gamma}} + (\mathbf{F}^p)^{-1} \overset{(e)}{\mathbf{\Gamma}}_\mathcal{K} [\mathbf{F}^p, \mathbf{F}^p], \quad \mathbf{\Gamma} = \mathbf{F}^{-1}\nabla\mathbf{F}. \end{aligned} \tag{8}$$

Here the plastic connection with respect to the configuration with torsion, $\overset{(p)}{\mathbf{\Gamma}}_\mathcal{K}$, is related with the plastic connection, $\overset{(p)}{\mathbf{\Gamma}}$, previously defined with respect to the reference configuration, by the following relationships

$$\overset{(p)}{\mathbf{\Gamma}}_\mathcal{K} = -\mathbf{F}^p \overset{(p)}{\mathbf{\Gamma}} [(\mathbf{F}^p)^{-1}, (\mathbf{F}^p)^{-1}]. \tag{9}$$

The plastic metric tensor $\mathbf{C}^p$ and strain gradient $\mathbf{C}$ are defined with respect to the reference configuration, while the elastic metric tensor $\mathbf{C}^e$ is defined in configuration with torsion by

$$\mathbf{C}^p := (\mathbf{F}^p)^T\mathbf{F}^p, \quad \mathbf{C}^e = (\mathbf{F}^p)^{-T}\mathbf{C}(\mathbf{F}^p)^{-1}, \quad \mathbf{C} = \mathbf{F}^T\mathbf{F}. \tag{10}$$

Definition 2.1. *The Bilby's type plastic connection is defined in a coordinate system through*

$$\overset{(p)}{\mathbf{A}} := (\mathbf{F}^p)^{-1}\nabla\mathbf{F}^p. \tag{11}$$

Remark 2.1. *The Cartan torsion that belongs to the Bilby's connection is given by* $(\mathbf{Su})\mathbf{v} = (\mathbf{F}^p)^{-1}(((\nabla\mathbf{F}^p)\mathbf{u})\mathbf{v} - ((\nabla\mathbf{F}^p)\mathbf{u})\mathbf{v})$, *while the curvature tensor is vanishing. Moreover, if the second order torsion tensor* $\mathcal{N}$ *is defined by* $\mathcal{N}(\mathbf{u}\times\mathbf{v}) = (\mathbf{Su})\mathbf{v}$, *then it has the representation* $\mathcal{N} = (\mathbf{F}^p)^{-1} curl\mathbf{F}^p$. *Consequently, we can say that the torsion tensor* $\mathcal{S}$ *is equivalent to* $curl\mathbf{F}^p$.

Let us introduce the expression for the plastic connection with respect to the reference configuration built by Cleja-Tigoiu in [5], which has metric property with respect to $\mathbf{C}^p$, and that allows a represented under the form

$$\overset{(p)}{\mathbf{\Gamma}} = \overset{(p)}{\mathcal{A}} + (\mathbf{C}^p)^{-1}(\mathbf{\Lambda}\times\mathbf{I}), \tag{12}$$

where the third order tensor $\mathbf{\Lambda} \times \mathbf{I}$, generated by the second order (covariant) tensor $\mathbf{\Lambda}$ is defined by (4), namely

$$((\mathbf{\Lambda} \times \mathbf{I})\mathbf{u})\mathbf{v} = \mathbf{\Lambda u} \times \mathbf{v}, \quad \forall\, \mathbf{u}, \mathbf{v} \in \mathcal{V}. \tag{13}$$

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

3. SCREW DISLOCATION

First the *skew dislocation* will be defined in connection with the definition of the Burgers vector. The Burgers vector can be defined in terms of the plastic distortion $\mathbf{F}^p$, by considering a closed curve (*circuit*) C_0 in the reference configuration of the body and $\mathcal{A}_0$ a surface with normal $\mathbf{N}$ bounded by C_0

$$\mathbf{b} = \int_{C_0} \mathbf{F}^p \, d\mathbf{X} = \int_{\mathcal{A}_0} (\mathrm{curl}(\mathbf{F}^p))\mathbf{N} dA = \int_{\mathcal{A}_\mathcal{K}} \boldsymbol{\alpha}_\mathcal{K} \mathbf{n}_\mathcal{K} dA_\mathcal{K}, \tag{14}$$

where $\boldsymbol{\alpha}_\mathcal{K}$ is Noll's dislocation density in [13]

$$\boldsymbol{\alpha}_\mathcal{K} \equiv \frac{1}{\det \mathbf{F}^p}(\mathrm{curl}(\mathbf{F}^p))(\mathbf{F}^p)^T. \tag{15}$$

The expression of the Burgers vector can be aproximate by the formula

$$\mathbf{b} \simeq \mathrm{curl}(\mathbf{F}^p)\mathbf{N}\ \mathrm{area}(\mathcal{A}_0). \tag{16}$$

In crystal plasticity the presence of the defects inside the crystals is measured by non-vanishing Burgers vector. The integral representation (14) shows that non-zero *curl* of plastic distortion, supposed to be continuum and non-zero in a certain material neighborhood, leads to a non-vanishing Burgers vector.

Definition 3.1. *We say that the plastic distortion* $\mathbf{F}^p$ *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.* $\mathbf{b} \parallel \mathbf{N}$, *in contrast with the edge dislocation when* $\mathbf{b} \perp \mathbf{N}$.

Let us introduce a Cartesian basis $(\mathbf{e}_1, \quad \mathbf{e}_2, \quad \mathbf{e}_3)$ and a plastic distortion $\mathbf{F}^p$ which defines a *screw dislocation* that correspond to a Burgers vector directed to $\mathbf{e}_3$, given by

$$\begin{aligned} &\mathbf{F}^p = \mathbf{I} + \mathbf{e}_3 \otimes \boldsymbol{\tau}, \quad \boldsymbol{\tau} \perp \mathbf{e}_3, \quad \text{with} \\ &\boldsymbol{\tau} : \mathcal{D} \subset R^2 \longrightarrow \mathcal{V}, \quad \boldsymbol{\tau} := F^p_{31}\mathbf{e}_1 + F^p_{32}\mathbf{e}_2, \quad J^p := det(\mathbf{F}^p) = 1. \end{aligned} \tag{17}$$

The mathematical description of the problem related to the screw dislocation within the finite elasticity is performed by Cermelli and Gurtin [2].

If we consider that $\boldsymbol{\tau} = \boldsymbol{\tau}(x^1, x^2)$, the *curl* of the plastic distortion, see (1), is given by

$$\mathrm{curl}\ \mathbf{F}^p = \Big(\frac{\partial F^p_{31}}{\partial x^2} - \frac{\partial F^p_{32}}{\partial x^1}\Big)\ \mathbf{e}_3 \otimes \mathbf{e}_3, \tag{18}$$

and Bilby's type plastic connection

$$\overset{(p)}{\mathbf{A}} := (\mathbf{F}^p)^{-1}\nabla\mathbf{F}^p = \mathbf{e}_3 \otimes \nabla\boldsymbol{\tau}, \quad \nabla\boldsymbol{\tau} = \frac{\partial\tau_\beta}{\partial x^\delta}\,\mathbf{e}_\beta \otimes \mathbf{e}_\delta, \quad \beta, \delta \in \{1, 2\}. \tag{19}$$

The representation given in (18) justifies the name attributed to the plastic distortion introduced in (17), taking into account the expression for the Burgers vector, for a plane curve with the normal $\mathbf{e}_3$.

Let us remark its appropriate *trace* $\mathrm{tr}_{(2)}\,\overset{(p)}{\mathbf{A}}$, defined by the formula (5)

$$\mathrm{tr}_{(2)}\,\overset{(p)}{\mathbf{A}}\cdot\mathbf{u} := \mathrm{tr}(\overset{(p)}{\mathbf{A}}\,\mathbf{u}) = \mathrm{tr}((\mathbf{e}_3 \otimes \nabla\boldsymbol{\tau})\mathbf{u}) = \mathbf{e}_3\nabla\boldsymbol{\tau}(\mathbf{u}) = \frac{\partial\boldsymbol{\tau}_3}{\partial\mathbf{x}^\mathbf{k}}\mathbf{u}^\mathbf{k} = \mathbf{0}, \tag{20}$$

is zero, since $\tau_3 : \boldsymbol{\tau}\cdot\mathbf{e}_3 = 0$, $\boldsymbol{\tau}$ being a vector function orthogonal on $\mathbf{e}_3$.

The plastic metric tensor $\mathbf{C}^p$ has the representation

$$\mathbf{C}^p = \mathbf{I} + \boldsymbol{\tau} \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \boldsymbol{\tau} + \boldsymbol{\tau} \otimes \boldsymbol{\tau}. \tag{21}$$

Let us introduce the disclination tensor $\boldsymbol{\Lambda}$ represented in terms of Frank vector $\boldsymbol{\omega}$, like in Cleja-Ţigoiu [5]

$$\boldsymbol{\Lambda} := \eta\boldsymbol{\omega} \otimes \boldsymbol{\zeta}, \tag{22}$$

$\boldsymbol{\zeta}$ the tangent vector line for the disclination field, and the scalar valued function η have to be defined. It follows that

$$\nabla\boldsymbol{\Lambda} := \boldsymbol{\omega} \otimes \boldsymbol{\zeta} \otimes \nabla\eta, \quad \dot{\boldsymbol{\Lambda}} := \dot{\eta}\boldsymbol{\omega} \otimes \boldsymbol{\zeta}, \tag{23}$$

if we take constant value for $\boldsymbol{\zeta}$.

Hypothesis. We assume that Frank and Burgers vectors are orthogonal, $\boldsymbol{\omega}\cdot\mathbf{b} = 0$, here $\mathbf{b} = \mathbf{e}_3$. This hypothesis corresponds to the physical meaning attributed to these types of lattice defects. See for instance [3].

Remark 3.1. *In Fig.1 the Burgers vector produced by the screw dislocation and the rotation produced by the disclinations have been plotted, following the comments from [3].*

4. MACRO AND MICRO FORCES

Within the constitutive framework developed in [6], we consider that the free energy in the reference configuration can be introduce in terms of the deformation fields listed below

$$\psi = \psi(\mathbf{C}^e, \mathbf{F}^p, \overset{(p)}{\mathcal{A}}, \boldsymbol{\Lambda}, \nabla\boldsymbol{\Lambda}) \equiv \psi^{ev}(\mathbf{C}, \mathbf{F}^p, \overset{(p)}{\mathcal{A}}) + \psi^d(\boldsymbol{\Lambda}, \nabla\boldsymbol{\Lambda}), \tag{24}$$

but in contrast with [6] we have no influence of the elastic connection.

Concerning the free energy function we assume that the *defect energy* is given by

$$\psi^d(\nabla\boldsymbol{\Lambda}) = \frac{\kappa_2}{2}\beta_2^2\nabla\boldsymbol{\Lambda}\cdot\nabla\boldsymbol{\Lambda}, \tag{25}$$

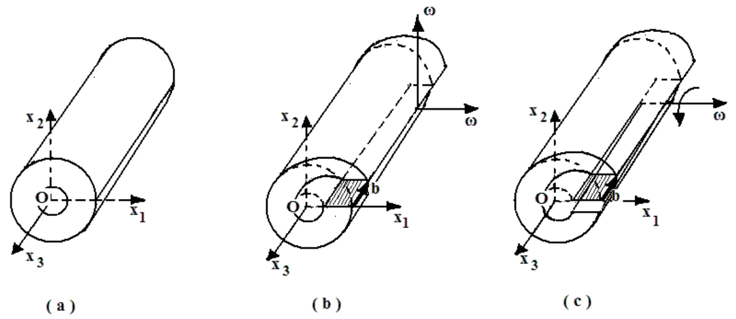

Fig. 1. Lattice defects: Screw dislocaton with Burgers vector **b**, disclination with Frank vector ω.

with β_2 a length scale parameter.

Ax.2 The macro forces are $\mathbf{T}-$ the non-symmetric Cauchy stress and macro stress momentum, $\boldsymbol{\mu}$, which is described by a third order tensor field, satisfy the macro *balance equation*

$$\text{div}\,\mathbf{T} + \rho\mathbf{b} = 0, \quad -2\mathbf{T}^a = \text{div}\,\boldsymbol{\mu}, \tag{26}$$

$\mathbf{T}^a$ is the skew symmetric part of the stress tensor. The equations (26) are similar to those proposed in Fleck et al. [8], see also Cleja-Tigoiu [4], [6]

We denote by $\rho, \tilde{\rho}, \rho_0$ the mass densities in the actual configuration, in the configuration with torsion and in the reference one.

When we pull back the macro stress $\boldsymbol{\mu}$ to the configuration with torsion, the appropriate expression for the macro stress momentum $\boldsymbol{\mu}_{\mathcal{K}}$ is derived

$$\frac{1}{\tilde{\rho}_0}\boldsymbol{\mu}_{\mathcal{K}} := (\mathbf{F}^e)^T \frac{1}{\tilde{\rho}}\boldsymbol{\mu}[(\mathbf{F}^e)^{-T}, (\mathbf{F}^e)^{-T}], \quad \text{where} \quad \mathbf{F}^e = \mathbf{F}(\mathbf{F}^p)^{-1}. \tag{27}$$

Ax.3 The micro stress denoted by $\boldsymbol{\Upsilon}^\lambda$ and micro momentum respectively, denoted by $\boldsymbol{\mu}^\lambda$, which are associated with the disclinations satisfy in $\mathcal{K}$ their own balance equation (see [6]):

$$\boldsymbol{\Upsilon}^\lambda = \text{div}_{\mathcal{K}}\,\boldsymbol{\mu}^\lambda + \tilde{\rho}\mathbf{B}^\lambda \quad \Longleftrightarrow \quad J^p\,\boldsymbol{\Upsilon}^\lambda = \text{div}\,(J^p\,\boldsymbol{\mu}^\lambda(\mathbf{F}^p)^{-T}) + \tilde{\rho}\mathbf{B}^\lambda. \tag{28}$$

Here $\tilde{\rho}\mathbf{B}^\lambda$ is mass density of the couple body force, $J^p = \mid det\mathbf{F}^p \mid$.

Ax.4 The micro stress $\boldsymbol{\Upsilon}^p$ and micro stress momentum $\boldsymbol{\mu}^p$ are associated with the plastic mechanism, and they satisfy their own balance equation in the configuration with torsion $\mathcal{K}$:

$$
\begin{aligned}
&\boldsymbol{\Upsilon}^p = \mathrm{div}_{\mathcal{K}}\,(\boldsymbol{\mu}^p - \boldsymbol{\mu}_{\mathcal{K}}) + \tilde{\rho}\mathbf{B}^\lambda \quad \Longleftrightarrow \\
&J^p\,\boldsymbol{\Upsilon}^p = \mathrm{div}\,(J^p\,(\boldsymbol{\mu}^p - \boldsymbol{\mu}_{\mathcal{K}})(\mathbf{F}^p)^{-T}) + \tilde{\rho}\mathbf{B}^p.
\end{aligned}
\tag{29}
$$

Here $\tilde{\rho}\mathbf{B}^p$ is appropriate mass density of the couple body force.The equation (29) could be found in a modified form in [5].

The constitutive restrictions imposed by the free energy imbalance, that have been obtained by Cleja-Ţigoiu in [6], are adapted to the proposed here model as it follows.

The elastic type constitutive functions are derived from the free energy function, viewed like a potential for Cauchy stress

$$
\frac{1}{\rho}\mathbf{T} = 2\mathbf{F}(\partial_{\mathbf{C}}\psi)\mathbf{F}^T, \quad \boldsymbol{\mu} = \partial_{\boldsymbol{\Gamma}}\psi, \tag{30}
$$

but here $\boldsymbol{\mu} = 0$, as a consequence of the supposition made in (24) that the free energy function is not dependent on $\boldsymbol{\Gamma}$.

We postulate here an energetic (non-dissipative) constitutive equation for the micro stress momentum associated with plastic behaviour and disclinations, respectively

$$
\begin{aligned}
&\frac{1}{\rho_0}\boldsymbol{\mu}_0{}^p = \partial_{\underset{\mathcal{A}}{(\mathrm{p})}}\psi \\
&\frac{1}{\rho_0}\boldsymbol{\mu}_0^\lambda = \partial_{\nabla\boldsymbol{\Lambda}}\psi^d(\nabla\boldsymbol{\Lambda}) = \kappa_2\beta_2^2\,\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta.
\end{aligned}
\tag{31}
$$

The last equality is a consequence of (25) together with (23).

The expressions for the micro stress plastic momentum $\boldsymbol{\mu}^p$ and the macro stress momentum $\boldsymbol{\mu}_{\mathcal{K}}$ both of them being considered with respect to $\mathcal{K}$, pulled back to the reference configuration cab be expressed under the form

$$
\begin{aligned}
&\frac{1}{\rho_0}\boldsymbol{\mu}_0^p := (\mathbf{F}^p)^T\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p[(\mathbf{F}^p)^{-T}, (\mathbf{F}^p)^{-T}], \\
&\frac{1}{\rho_0}\boldsymbol{\mu}_0 := (\mathbf{F}^p)^T\frac{1}{\tilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}}[(\mathbf{F}^p)^{-T}, (\mathbf{F}^p)^{-T}],
\end{aligned}
\tag{32}
$$

as well as the micro stress momentum associated with the disclination in $\mathcal{K}$ can be expressed in terms of $\boldsymbol{\mu}_0^\lambda$ by

$$
\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^\lambda := (\mathbf{F}^p)^{-T}\frac{1}{\tilde{\rho}_0}\boldsymbol{\mu}_0^\lambda[(\mathbf{F}^p)^T, (\mathbf{F}^p)^T]. \tag{33}
$$

The *viscoplastic type, dissipative evolution equations* for plastic distorsion $\mathbf{F}^p$ and $\boldsymbol{\Lambda}$ have been postulated in [6] to be compatible with the appropriate dissipation inequality. The viscoplastic evolution equation for plastic distortion, giving rise to the rate of plastic distortion with respect to the reference configuration is given by

$$\begin{aligned} &\mathbf{l}^p = -(\mathbf{F}^p)^{-1}\dot{\mathbf{F}}^p \\ &\frac{1}{\rho_0}(\mathbf{\Sigma}_0 - \mathbf{\Sigma}_0{}^p) + (\mathbf{F}^p)^T \partial_{\mathbf{F}^p}\psi = \xi_1 \, \mathbf{l}^p. \end{aligned} \tag{34}$$

Definition 4.1. *The Mandel type stress measures in the reference configuration are associated with the appropriate stresses as it follows*

$$\frac{1}{\rho_0}\mathbf{\Sigma}_0^p = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^T \mathbf{\Upsilon}^p (\mathbf{F}^p)^{-T}, \quad \frac{1}{\rho_0}\mathbf{\Sigma}_0 = \frac{1}{\rho}\mathbf{F}^T\mathbf{T}\mathbf{F}^{-T} \tag{35}$$

and

$$\frac{1}{\rho_0}\mathbf{\Sigma}_0^\lambda = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^T \mathbf{\Upsilon}^\lambda (\mathbf{F}^p)^{-T}. \tag{36}$$

The *viscoplastic type, dissipative evolution equations* are postulated for disclination $\mathbf{\Lambda}$

$$\begin{aligned} &(\frac{1}{\rho_0}\mathbf{\Sigma}_0{}^\lambda - \partial_{\mathbf{\Lambda}}\,\psi) + (\overset{(p)}{\mathcal{A}} \odot \frac{1}{\rho_0}\boldsymbol{\mu}_0^\lambda) - \\ &-(\frac{1}{\rho_0}\boldsymbol{\mu}_0^\lambda \, {}_r\!\odot \overset{(p)}{\mathcal{A}}\,) - \frac{1}{\rho_0}\boldsymbol{\mu}_0^\lambda(\mathrm{tr}_{(2)}(\overset{(p)}{\mathcal{A}})) = \xi_3 \, \dot{\mathbf{\Lambda}}. \end{aligned} \tag{37}$$

Ax.5 The scalar constitutive functions ξ_1, ξ_3 are defined in such a way to be compatible with the dissipation inequality

$$\xi_1 \, \mathbf{l}^p \cdot \mathbf{l}^p + \xi_3 \, \dot{\mathbf{\Lambda}} \cdot \dot{\mathbf{\Lambda}} \geq 0. \tag{38}$$

Note that the dissipation inequality is reduced to the expression written in the left hand side of (39) if the viscoplastic type equations (34) and (38) have been accepted. The Mandel type stress measure associated with the disclination mechanism, $\mathbf{\Sigma}_0{}^\lambda$, is related to the micro stress $\mathbf{\Upsilon}^\lambda$ via (37), while $\boldsymbol{\mu}_0^\lambda$ is expressed in (31).

5. DISCLINATIONS GENERATED BY A PLASTIC DISTORTION

We suppose that the second order disclination tensor $\mathbf{\Lambda}$ is described in terms of Frank vector $\boldsymbol{\omega}$, with the scalar intensity function η and the disclination line $\boldsymbol{\zeta}$, say constant during the deformation process, have to be found.

We are now able to solve **the problem**: Find the disclination tensor $\mathbf{\Lambda}$, having the expression (22), to be solution of the evolution equation (38) with the micro stresses related by (37), and which is compatible with the micro balance equation associated with the disclination, $(28)_2$.

We take into account the physically motivated hypothesis that the Frank and Burgers vectors are (fixed) orthogonal, as well as that the plastic distorsion (17) characterizes the *screw dislocation*, then

$$\boldsymbol{\omega} \cdot \mathbf{e}_3 = 0, \quad \boldsymbol{\tau} \cdot \mathbf{e}_3 = 0, \quad \nabla(\boldsymbol{\tau})\mathbf{u} \cdot \mathbf{e}_3 = 0, \quad \forall \quad \mathbf{u} \in \mathcal{V}. \tag{39}$$

First of all we eliminate the micro stress from (38), via (28) together with (37).

By definitions and the hypotheses, from (33) together with $(31)_2$ we get

$$\boldsymbol{\mu}^{\lambda}(\mathbf{F}^{p})^{-T} = \rho_0(\mathbf{F}^{p})^{-T}\partial_{\nabla\boldsymbol{\Lambda}}\psi[\mathbf{I},(\mathbf{F}^{p})^{T}]. \tag{40}$$

As a direct consequence of (24) together with (25) and (23) we can prove the following relationship

$$\frac{1}{\rho_0}\boldsymbol{\mu}^{\lambda}(\mathbf{F}^{p})^{-T} = \kappa_2\beta_2^2\,\{\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta + (\boldsymbol{\zeta}\cdot\mathbf{e}_3)(\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta)\}. \tag{41}$$

Consequently, we apply the *divergence operator* to (42) and then

$$\begin{aligned} \operatorname{div}\,(\,\boldsymbol{\mu}^{\lambda}(\mathbf{F}^{p})^{-T}) &= \kappa_2\beta_2^2\rho_0\;\Delta\eta\{\boldsymbol{\omega}\otimes\boldsymbol{\zeta} + (\boldsymbol{\zeta}\cdot\mathbf{e}_3)\;\boldsymbol{\omega}\otimes\boldsymbol{\tau}\}+ \\ &+\kappa_2\beta_2^2\rho_0(\boldsymbol{\zeta}\cdot\mathbf{e}_3)\;(\boldsymbol{\omega}\otimes((\nabla\;\boldsymbol{\tau})\nabla\eta) \end{aligned} \tag{42}$$

holds. Here $\Delta\eta$ denotes the Laplacean of the scalar function η.

Proposition 5.1. *In the evolution equation for* $\boldsymbol{\Lambda}$, *written in (38) the term*

$$(\overset{(p)}{\mathcal{A}}\odot\frac{1}{\rho_0}\boldsymbol{\mu}_0^{\lambda}) = \kappa_2\beta_2^2\;(\mathbf{e}_3\otimes\nabla\boldsymbol{\tau})\odot(\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta), \tag{43}$$

is vanishing, since its components are given by

$$(\overset{(p)}{\mathcal{A}}\odot\frac{1}{\rho_0}\boldsymbol{\mu}_0^{\lambda})_{sn} = \kappa_2\beta_2^2\;(\mathbf{e}_s\cdot\boldsymbol{\zeta})(\mathbf{e}_n\cdot(\nabla\boldsymbol{\tau})\nabla\eta)(\mathbf{e}_3\cdot\boldsymbol{\omega}) = 0, \tag{44}$$

while the following expression

$$(\frac{1}{\rho_0}\boldsymbol{\mu}_0^{\lambda}\;{}_r\!\odot\overset{(p)}{\mathcal{A}}\;) = \kappa_2\beta_2^2\;(\boldsymbol{\zeta}\cdot(\nabla\boldsymbol{\tau})\nabla\eta)\;\mathbf{e}_3\otimes\boldsymbol{\omega}. \tag{45}$$

has to be introduced inside.

In order to **prove** the above relationships we calculate the components of the second order tensor field, starting from the definitions introduced in (6). The scalar product of the tensor written in the left hand side of (44) with $(\mathbf{e}_n\otimes\mathbf{e}_s)$ gives rise to the components sn of the tensor. We perform the tensorial operations and we arrive at

$$\begin{aligned} &\kappa_2(\beta_2)^2((\mathbf{e}_3\otimes\nabla\boldsymbol{\tau})\;\odot(\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta))\cdot(\mathbf{e}_n\otimes\mathbf{e}_s) = \\ &= \kappa_2(\beta_2)^2\;(\mathbf{e}_3\otimes\nabla\boldsymbol{\tau})[\mathbf{I},\mathbf{e}_n\otimes\mathbf{e}_s]\;\cdot(\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta) = \\ &= \kappa_2(\beta_2)^2\;(\mathbf{e}_3\otimes\mathbf{e}_s\otimes(\nabla\boldsymbol{\tau})^{T}\mathbf{e}_n)\;\cdot(\boldsymbol{\omega}\otimes\boldsymbol{\zeta}\otimes\nabla\eta) = \\ &= \kappa_2(\beta_2)^2\;(\mathbf{e}_3\otimes\boldsymbol{\omega})(\mathbf{e}_s\cdot\boldsymbol{\zeta})\mathbf{e}_n\cdot((\nabla\boldsymbol{\tau})\nabla\eta). \end{aligned} \tag{46}$$

Note the formula proved below via (3) has been used in the previously written expression, namely

$$\begin{aligned}(\mathbf{e}_3 \otimes \nabla\boldsymbol{\tau})[\mathbf{I}, \mathbf{e}_n \otimes \mathbf{e}_s]\mathbf{u} &= (\mathbf{e}_3 \otimes (\nabla\boldsymbol{\tau})\mathbf{u})(\mathbf{e}_n \otimes \mathbf{e}_s) = \\ &= (\mathbf{e}_3 \otimes \mathbf{e}_s)(\nabla\boldsymbol{\tau})\mathbf{u} \cdot \mathbf{e}_n) = (\mathbf{e}_3 \otimes \mathbf{e}_s \otimes (\nabla\boldsymbol{\tau})\mathbf{e}_n)\mathbf{u},\end{aligned} \tag{47}$$

hold for all $\mathbf{u} \in \mathcal{V}$, since $\nabla\boldsymbol{\tau} \in Lin$.
We proceed similarly to the calculus of the term written in the left hand side of (46). We take the scalar product with $(\mathbf{e}_n \otimes \mathbf{e}_s)$ and we use the definitions introduced in (6)

$$\begin{aligned}&(\frac{1}{\rho_0}\boldsymbol{\mu}_0^\lambda \,_r\odot \overset{(\mathrm{p})}{\mathcal{A}}\,) \cdot (\mathbf{e}_n \otimes \mathbf{e}_s) = \\ &= \kappa_2\beta_2^2\,(\boldsymbol{\zeta} \cdot (\nabla\boldsymbol{\tau})\nabla\eta) \cdot (\mathbf{e}_n \otimes \mathbf{e}_s)\,\overset{(\mathrm{p})}{\mathcal{A}},\end{aligned} \tag{48}$$

as well as the formula

$$(\mathbf{e}_n \otimes \mathbf{e}_s)\,(\mathbf{e}_3 \otimes \nabla\boldsymbol{\tau}) = \delta_{3s}\mathbf{e}_n \otimes \nabla\boldsymbol{\tau}. \tag{49}$$

We use the balance equation for micro forces associated with the dislocation (28) composed on the left with $(\mathbf{F}^p)^T = \mathbf{I} + \boldsymbol{\tau} \otimes \mathbf{e}_3$ and on right with $(\mathbf{F}^p)^{-T} = \mathbf{I} - \boldsymbol{\tau} \otimes \mathbf{e}_3$ in order to express the Mandel's type stress tensor (37)

$$\begin{aligned}&\frac{1}{\rho_0}\boldsymbol{\Sigma}_0^\lambda = \kappa_2\beta_2^2\,\{\Delta\eta(\boldsymbol{\omega} \otimes \boldsymbol{\zeta} + (\boldsymbol{\zeta} \cdot \mathbf{e}_3)\boldsymbol{\omega} \otimes \boldsymbol{\tau}) + \\ &+(\boldsymbol{\zeta} \cdot \mathbf{e}_3)\boldsymbol{\omega} \otimes ((\nabla\boldsymbol{\tau})\nabla\eta)\} - \kappa_2\beta_2^2\,\Delta\eta(\boldsymbol{\zeta} \cdot \boldsymbol{\tau})(\boldsymbol{\omega} \otimes \mathbf{e}_3) - \\ &-\kappa_2\beta_2^2\,\Delta\eta(\boldsymbol{\zeta} \cdot \mathbf{e}_3)\{\Delta\eta \mid \boldsymbol{\tau} \mid^2 + ((\nabla\boldsymbol{\tau})\nabla\eta) \cdot \boldsymbol{\tau}\}\boldsymbol{\omega} \otimes \mathbf{e}_3.\end{aligned} \tag{50}$$

Proposition 5.2. *The evolution equation for* $\boldsymbol{\Lambda}$ *written in (38) becomes*

$$\frac{1}{\rho_0}\boldsymbol{\Sigma}_0{}^\lambda - \kappa_2\beta_2^2\,(\boldsymbol{\zeta} \cdot (\nabla\boldsymbol{\tau})\nabla\eta)\,\mathbf{e}_3 \otimes \boldsymbol{\omega} = \xi_3\,\dot{\eta}\boldsymbol{\omega} \otimes \boldsymbol{\zeta}, \tag{51}$$

where the first term is given by (51), since $tr_{(2)}\,\overset{(\mathrm{p})}{\mathcal{A}} = 0$.

We investigate now the consequences that follows from (52) and (51).
If $\boldsymbol{\zeta} \cdot \mathbf{e}_3 = 0$, the projection on $\boldsymbol{\zeta}$ of the equation (52) together with (51) leads to

$$\xi_3\dot{\eta} = \kappa_2\beta_2^2\Delta\eta. \tag{52}$$

When we return to the equation (52), we conclude that the following conditions

$$(\boldsymbol{\zeta} \cdot \boldsymbol{\tau})\Delta\eta = 0, \quad \boldsymbol{\zeta} \cdot \nabla\boldsymbol{\tau})\nabla\eta = 0 \tag{53}$$

necessarily hold.

If $\boldsymbol{\zeta}\cdot\mathbf{e}_3 \neq 0$, as $\boldsymbol{\omega}\cdot\mathbf{e}_3 = 0, \boldsymbol{\tau}\cdot\mathbf{e}_3 = 0$, the projection of the evolution equation on the Burgers vector, here on $\mathbf{e}_3$, is reduced to

$$\begin{aligned}&+\kappa_2\beta_2^2\,(\,-\,\Delta\eta\,(\boldsymbol{\zeta}\cdot\boldsymbol{\tau})\boldsymbol{\omega} + (\boldsymbol{\zeta}\cdot\mathbf{e}_3)\{(1-\mid\boldsymbol{\tau}\mid^2)\Delta\eta- \\ &-((\nabla\boldsymbol{\tau})\nabla\eta)\cdot\boldsymbol{\tau}\}\boldsymbol{\omega}) = \xi_3\,\dot{\eta}(\boldsymbol{\zeta}\cdot\mathbf{e}_3)\boldsymbol{\omega}.\end{aligned} \tag{54}$$

If we restrict to the condition $\zeta = \mathbf{e}_3$, the equation (55) becomes

$$\kappa_2\beta_2^2\,\{\Delta\eta(1-\mid\boldsymbol{\tau}\mid^2) - ((\nabla\boldsymbol{\tau})\nabla\eta)\cdot(\boldsymbol{\tau})\} = \xi_3\,\dot{\eta}. \tag{55}$$

When we return to the equation (51) together with (50) the compatibility condition

$$\Delta\eta\,\boldsymbol{\tau} + (\nabla\boldsymbol{\tau})\nabla\eta = 0 \tag{56}$$

follows. We consider the scalar product of (57) with $\boldsymbol{\tau}$ and we arrive at the equality

$$\Delta\eta\ \mid\boldsymbol{\tau}\mid^2 + \boldsymbol{\tau}\cdot((\nabla\boldsymbol{\tau})\nabla\eta) = 0. \tag{57}$$

Note that the equation (56) together with (58) becomes (53). Thus we proved the following result.

Theorem 5.1. *Let us assume that* $\mathbf{e}_3\cdot\boldsymbol{\omega} = 0$.

1 *If the disclination line* ζ *is orthogonal to the Burgers vector, namely* $\mathbf{e}_3\cdot\boldsymbol{\zeta} = 0$ *the evolution equation for the density of disclination is given by*

$$\xi_3\dot{\eta} = \kappa_2\beta_2^2\Delta\eta, \tag{58}$$

and the compatibility condition is reduced to $\boldsymbol{\zeta}\cdot\boldsymbol{\tau} = 0$.

2 *If the disclination line is collinear with Burgers vector, i.e.* $\boldsymbol{\zeta} \parallel \mathbf{e}_3$, *the evolution equation for the disclination intensity is still given by (59), while the compatibility condition, namely between the plastic distortion expressed in terms of* $\boldsymbol{\tau}$ *and* η, *is derived under the form*

$$\boldsymbol{\tau}\Delta\eta + (\nabla\boldsymbol{\tau})\nabla\eta = 0. \tag{59}$$

6. CONCLUSIONS

In **Theorem 5.1** under the assumption that the plastic distortion is described by a screw dislocation we derived the non-local evolution for scalar disclination density. We assumed that the disclination is described in terms of Frank vector and disclination line. If the Frank and Burgers vectors are orthogonal, and moreover the dislocation and the disclination lines are either collinear, or perpendicular one to the another, then the evolution of scalar disclination density η is not influenced by the evolution of plastic distorsion. A non-local evolution equation for η is derived. The result is similar with those obtained in [6], for the case of plastic shear distortion, but there the directions of the Frank vector and the Burgers vector could be arbitrarily given. The same type of the analysis can be conducted for the edge dislocation.

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