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THE INFLUENCE OF DISLOCATION DENSITY ON THE BEHAVIOUR OF CRYSTALLINE MATERIALS

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Abstract. An elasto-plastic constitutive model is proposed to describe the behaviour of crystalline materials with microstructural defects like dislocations. The defects are defined in terms of the incompatible plastic distortion. The model involves the free energy assumed to be dependent on the elastic strain and torsion of the Bilby connection. The non-local diffusion-like evolution equation describing the plastic distortion is derived. In the case of small distortions, the edge dislocations are defined and the evolution equation for the plastic distortion tensor is derived starting from the finite distortion case. The initial and boundary value problem concerning the tensile test of a non-rectangular sheet is solved numerically in the hypothesis that, at the initial moment, a single area of dislocations describes the heterogeneity of defects.

Key words: Burger vector, dislocation density, diffusion-like evolution for plastic distortion, variational equality, FEM and update algorithm.

1. INTRODUCTION

In this paper, we present a model within the constitutive framework proposed in [10], by considering dislocations only as defects, without disclinations. The results provided here appear as particular cases of those obtained in the above mentioned paper.

The measures of defects are defined in terms of the incompatible *plastic distortion*, $\mathbf{F}^p$. The defect densities characterize the Burgers vectors defined within the finite deformation framework, and are reduced to $\operatorname{curl} \mathbf{H}^p$ in the case of small plastic distortion. Comparing to [8] where the scalar densities of dislocations in slip systems have been considered, in the present model we adopt tensorial densities of dislocations. Also, in [8, 9] non-local diffusion-type equations for scalar densities of dislocations were represented. In the numerical example presented in [7], at the initial moment, a non-homogeneous distribution of the scalar densities of dislocations was assumed, only the local type of the evolution equations being considered.

In Section 2 we recall the definition of the Burgers vector, and tensorial definitions for the dislocation densities. In Section 3 the principle of the free energy imbalance is formulated like in [5] (following the idea of Gurtin [14, 1]. The viscoplastic-like equation for micro forces and a new evolution equation for the plastic distortion were derived, with respect to the reference configuration within the large deformation formalism. In Section 4 we restrict to the small elasto-plastic distortions formalism and the evolution equation is also provided.

In section 5, the corresponding variational equalities for the incremental equilibrium equation, and the evolution equation for the plastic distortion were formulated. In Section 6 we consider a tensile problem in a non-rectangular sheet when dislocations describe the initial heterogeneity of the defects. The initial and boundary value *problem is formulated.*

Notations. For a second-order tensor $\mathbf{A} \in \mathrm{Lin}$ and a third-order tensor $\boldsymbol{\Gamma} \in \mathrm{Lin}(\mathcal{V}, \mathrm{Lin}) \equiv \{\mathbf{N} : \mathcal{V} \to \mathrm{Lin},\ \text{linear}\}$, we denote: $(\nabla \mathbf{A})_{ijk} = \dfrac{\partial A_{ij}}{\partial X^k}$ the gradient components of the field

$\mathbf{A}$; $\mathrm{Skw}\boldsymbol{\Gamma}$ is defined by $((\mathrm{Skw}\boldsymbol{\Gamma})\mathbf{u})\mathbf{v} = (\boldsymbol{\Gamma}\mathbf{u})\mathbf{v} - (\boldsymbol{\Gamma}\mathbf{v})\mathbf{u}, \quad \forall\, \mathbf{u},\mathbf{v} \in \mathcal{V}$; $\mathrm{curl}\mathbf{A}$ is defined by $(\mathrm{curl}\mathbf{A})_{pi} = \varepsilon_{ijk} \dfrac{\partial A_{pk}}{\partial X^j}$, where ε_{ijk} denote Ricci permutation tensor components; The gradient with respect to the configuration with torsion $\mathcal{K}$ is given by $(\nabla_{\mathcal{K}}\mathbf{A})\tilde{\mathbf{u}} = (\nabla\mathbf{A})(\mathbf{A})^{-1}\tilde{\mathbf{u}}, \quad \forall \tilde{\mathbf{u}} \in \mathbf{F}^{\mathbf{p}}\mathcal{V}$; The second order velocity gradient is defined by $\left(\nabla_{\chi}\mathbf{L}\right)_{ijk} \equiv \dfrac{\partial}{\partial x^k}(\dfrac{\partial v_i}{\partial x^j})$, with $\mathbf{L} = \nabla_{\chi}\mathbf{v}$; $\boldsymbol{\Gamma}[\mathbf{F}_1,\mathbf{F}_2]$ is defined by $\left(\boldsymbol{\Gamma}[\mathbf{F}_1,\mathbf{F}_2]\mathbf{u}\right)\mathbf{v} = \left(\boldsymbol{\Gamma}(\mathbf{F}_1\mathbf{u})\right)\mathbf{F}_2\mathbf{v}, \forall\, \mathbf{u},\mathbf{v} \in \mathcal{V}$, where $\mathbf{F}_1$, $\mathbf{F}_2$ are second order tensors; $\{\mathbf{A}\}^S$, $\{\mathbf{A}\}^a$ are the symmetric and skew-symmetric parts of $\mathbf{A}$.

2. MEASURES OF DISLOCATIONS

The behaviour of elasto-plastic crystalline materials with defects is described in terms of three configurations: the reference configuration k of the body $\mathcal{B}$, $k(\mathcal{B}) \subset \mathcal{E}$, $\chi(\cdot,t)$ the deformed configuration at time t, for any motion of the body $\mathcal{B}$, $\chi : \mathcal{B} \times \mathbb{R} \to \mathcal{E}$ and the so-called current local relaxed configuration, or plastically deformed configurations $\mathcal{K}$.

The deformation gradient $\mathbf{F} = \nabla\chi(\mathbf{X},t)$ is *multiplicatively decomposed* into the elastic and plastic distortions, denoted by $\mathbf{F}^e$, $\mathbf{F}^p$, namely $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$, at every point of the body, using the physical arguments mentioned in [11]. The elastic and plastic distortions $\mathbf{F}^e$ and $\mathbf{F}^p$ are invertible tensors which *cannot be expressed* through *the gradient of certain vector fields.*

Let $\mathcal{A}_0$ be a surface with the normal $\mathbf{N}$ bounded by $\mathcal{C}_0$ a closed curve in the reference configuration. Following [4] the Burgers vector associated with the circuit $\mathcal{C}_0$ is defined by

$$\mathbf{b}_{\mathcal{K}} = \int_{\mathcal{C}_{\mathcal{K}}} \mathrm{d}\mathbf{x}_{\mathcal{K}} = \int_{\mathcal{C}_0} \mathbf{F}^p\, \mathrm{d}\mathbf{X} = \int_{\mathcal{A}_0} (\mathrm{curl}\mathbf{F}^p)\mathbf{N}\mathrm{d}A = \int_{\mathcal{A}_{\mathcal{K}}} \frac{1}{\det\mathbf{F}^p}(\mathrm{curl}\mathbf{F}^p)(\mathbf{F}^p)^{\mathrm{T}}\,\mathbf{n}_{\mathcal{K}}\mathrm{d}A_{\mathcal{K}}. \tag{1}$$

The *Noll's dislocation density tensor* $\boldsymbol{\alpha}_{\mathcal{K}}$ with respect to the configuration with torsion is expressed by $\boldsymbol{\alpha}_{\mathcal{K}} := \dfrac{1}{\det\mathbf{F}^p}(\mathrm{curl}\,\mathbf{F}^p)(\mathbf{F}^p)^{\mathrm{T}}$, and was introduced by [17]. By a pull-back procedure we define the dislocation density tensor $\boldsymbol{\alpha}$ with respect to the reference configuration $\boldsymbol{\alpha} := (\mathbf{F}^p)^{-1}\mathrm{curl}\mathbf{F}^p$.

We refer to the plastic distortion as *an incompatible field*. The plastic distortion has a non-vanishing curl, i.e. $\mathrm{curl}(\mathbf{F}^p) \neq 0$ in a material neighbourhood of the considered material point, which ensures the existence of a non-vanishing Burgers vector defined by the relation (1).

We define the *plastic Bilby connection* [3] in terms of the gradient of plastic distortion with respect to the reference configuration, k, by $\overset{(p)}{\mathcal{A}} = (\mathbf{F}^p)^{-1}\nabla\mathbf{F}^p$. Consequently, the tensorial measure of dislocation $\boldsymbol{\alpha}$ also means that $\boldsymbol{\alpha}(\mathbf{u}\times\mathbf{v}) = (\overset{(p)}{\mathcal{A}}\mathbf{u})\mathbf{v} - (\overset{(p)}{\mathcal{A}}\mathbf{v})\mathbf{u} = \left((\mathrm{Skw}\,\overset{(p)}{\mathcal{A}})\mathbf{u}\right)\mathbf{v}, \quad \forall\, \mathbf{u},\mathbf{v} \in \mathcal{V}$.

3. FREE ENERGY IMBALANCE AND MICRO BALANCE EQUATIONS. ELASTO-PLASTIC MODELS WITH DISLOCATIONS IN THE REFERENCE CONFIGURATION

3.1. Free energy imbalance

We assume the existence of the free energy density function and the definition of the internal power $(\mathcal{P}_{int})_{\mathcal{K}}$, which includes the work done by forces conjugated with the appropriate rate of second order elastic and plastic deformations. The effect of dislocations is involved in the model via the gradient of the plastic distortion.

AXIOM 1. *The elasto-plastic behaviour of the material is restricted to satisfy the free energy imbalance formulated in* $\mathcal{K}$ *and written for any virtual (isothermal) process, i.e.* $(\mathcal{P}_{int})_{\mathcal{K}} - \dot{\psi}_{\mathcal{K}} \geq 0.$

In the following $\rho_0, \tilde{\rho}, \rho$ are the mass densities in the initial, relaxed and actual configurations respectively, and they are related by $\tilde{\rho} J^p = \rho$, $\rho J = \rho_0$, where $J^p = \det \mathbf{F}^p$, $J = \det \mathbf{F}$.

AXIOM 2. *The internal power in* $\mathcal{K}$ *configuration is postulated to be given by*

$$(\mathcal{P}_{int})_{\mathcal{K}} = \frac{1}{\rho}\{\mathbf{T}\}^S \cdot \mathbf{L}^e + \frac{1}{\tilde{\rho}}\Upsilon^p \cdot \mathbf{L}^p + \frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p \cdot \nabla_{\mathcal{K}} \mathbf{L}^p + \frac{1}{\tilde{\rho}}\boldsymbol{\mu}_{\mathcal{K}} \cdot \left((\mathbf{F}^e)^{-1} (\nabla_{\chi} \mathbf{L})[\mathbf{F}^e, \mathbf{F}^e] - \nabla_{\mathcal{K}} \mathbf{L}^p \right). \tag{2}$$

Here the symmetric part $\{\mathbf{T}\}^S$ of the Cauchy stress tensor $\mathbf{T}$ is conjugate with the rate of elastic distortion, $\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}$, $\mathbf{L}^e = \dot{\mathbf{F}}^e (\mathbf{F}^e)^{-1}$, $\mathbf{L}^p = \dot{\mathbf{F}}^p (\mathbf{F}^p)^{-1}$. The macro stress momentum $\boldsymbol{\mu}_{\mathcal{K}}$, written in the last term of (2), is work conjugate with a measure of the gradient of the rate of elastic distortion. The micro forces $\left(\Upsilon^p, \boldsymbol{\mu}^p\right)$ are associated with the plastic behaviour.

Macro balance equations for the non-symmetric Cauchy stress, $\mathbf{T}$, and macro momentum $\boldsymbol{\mu}$ satisfy in the actual configuration the following balance equation

$$\operatorname{div}\left(\{\mathbf{T}\}^S - \frac{1}{2}\{\operatorname{div} \boldsymbol{\mu}\}^a \right) + \rho \mathbf{b} = 0. \tag{3}$$

We recall that the macro stress momenta, $\boldsymbol{\mu}$ and $\boldsymbol{\mu}_{\mathcal{K}}$, in the actual and anholonomic configuration are related by $\dfrac{\boldsymbol{\mu}}{\rho} = (\mathbf{F}^e)^{-\mathrm{T}} \dfrac{\boldsymbol{\mu}_{\mathcal{K}}}{\tilde{\rho}}[(\mathbf{F}^e)^{\mathrm{T}}, (\mathbf{F}^p)^{\mathrm{T}}]$.

For micro balance equations related to the plastic behaviour, we refer to [4,6].

PROPOSITION 1. *The micro balance equation for micro forces associated with the plastic mechanism is written in the reference configuration as*

$$J^p\, \Upsilon^p = \operatorname{div}(J^p\, (\boldsymbol{\mu}^p - \boldsymbol{\mu}_{\mathcal{K}})(\mathbf{F}^p)^{-\mathrm{T}}) + \rho_0 \mathbf{B}^p \ \ in\ \ \mathcal{B}^p, \quad \mu^p (\mathbf{F}^p)^{-\mathrm{T}} \mathbf{N} = \mathbf{M}^p \ \ on \ \ \partial \mathcal{B}^p. \tag{4}$$

In the following we postulate that the *free energy density* with respect to the reference configuration depends on the elastic strain and defects in the form $\psi = \frac{1}{4}\mathcal{E}(\mathbf{C} - \mathbf{C}^p)\cdot(\mathbf{C} - \mathbf{C}^p) + \frac{1}{2}\beta_2 \mathbf{S}^p \cdot \mathbf{S}^p$, where $\mathcal{E}$ is the elastic stiffness matrix, $\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}$, $\mathbf{C}^p = (\mathbf{F}^p)^{\mathrm{T}} \mathbf{F}^p$ and $\mathbf{S}^p$ is the skew-symmetric part of the connection $(\mathbf{S}^p \mathbf{u})\mathbf{v} \equiv \left((\operatorname{Skw} \overset{(p)}{\mathcal{A}})\mathbf{u} \right)\mathbf{v}$. Here β_2, is a real parameter.

The consequences induced by the principle of the free energy imbalance are the following:

PROPOSITION 2. 1. *The constitutive equations are reduced to the elastic constitutive one:*

$$\frac{1}{\rho}\{\mathbf{T}\}^S = 2\mathbf{F}\mathcal{E}(\mathbf{C} - \mathbf{C}^p)\mathbf{F}^{\mathrm{T}}, \ \frac{1}{\rho_0}\boldsymbol{\mu}_0 = \mathbf{0}, \tag{5}$$

and the energetic relationships which express the plastic micro momentum as

$$\frac{1}{\rho_0}\boldsymbol{\mu}_0^p = \beta_2 \mathbf{S}^p. \tag{6}$$

2. *The evolution equations for the plastic distortion are given by*:

$$\frac{1}{\rho_0}\mathbf{\Sigma}_0^p + 2\mathbf{C}^p\mathcal{E}(\mathbf{C}-\mathbf{C}^p) = \xi_1\overline{\mathbf{I}}^p, \text{ where } \overline{\mathbf{I}}^p = (\mathbf{F}^p)^{-1}\dot{\mathbf{F}}^p. \quad (7)$$

Here Mandel stress tensor, is introduced with respect to the reference configuration by $\frac{1}{\rho_0}\mathbf{\Sigma}_0^p = \frac{1}{\tilde{\rho}}(\mathbf{F}^p)^{\mathrm{T}}\mathcal{Y}^p(\mathbf{F}^p)^{-\mathrm{T}}$, while the micro stress momenta with respect to the reference configuration are expressed by $\frac{1}{\rho_0}\boldsymbol{\mu}_0^p = (\mathbf{F}^p)^{\mathrm{T}}\frac{1}{\tilde{\rho}}\boldsymbol{\mu}^p[(\mathbf{F}^p)^{-1},(\mathbf{F}^p)^{-1}]$.

4. MODEL WITH SMALL ELASTIC AND PLASTIC DISTORTIONS

Next, we consider the model of small distortions. In the case of small elastic and plastic distortions, the linearized expressions derived from the finite deformation fields are given by

$$\begin{aligned}&\mathbf{F} \simeq \mathbf{I}+\mathbf{H}, \quad \mathbf{H} = \nabla\mathbf{u}, \quad \boldsymbol{\varepsilon} = \{\mathbf{H}\}^S, \quad \mathbf{F}^p = \mathbf{I}+\mathbf{H}^p, \quad \overset{(p)}{\mathcal{A}} \simeq \nabla\mathbf{H}^p,\\ &\boldsymbol{\varepsilon}^p = \{\mathbf{H}^p\}^S, \quad \mathbf{C}-\mathbf{C}^p = 2(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^p), \quad \mathbf{C}^p = \mathbf{I}+2\boldsymbol{\varepsilon}^p,\end{aligned} \quad (8)$$

where $\mathbf{u}$ is the displacement vector. The torsion tensor $\mathbf{S}^p$ is expressed by $\mathbf{S}^p = \mathrm{Skw}\nabla\mathbf{H}^p$.

The energetic constitutive equations are given by

$$\frac{1}{\rho}\mathbf{T} = \mathcal{E}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^p), \quad \frac{1}{\rho}\boldsymbol{\mu}^p = \beta_2\,\mathrm{Skw}\nabla\mathbf{H}^p. \quad (9)$$

The micro forces are characterized by $\frac{1}{\rho_0}\mathbf{\Sigma}_0^p = \mathrm{div}(\frac{1}{\rho}\boldsymbol{\mu}^p) = -\beta_2\,\mathrm{curl}(\mathrm{curl}\mathbf{H}^p)$ as a consequence of its own balance equation (4).

Under the hypothesis of small distortions, the elasto-plastic problem is characterized, in terms of the displacement vector $\mathbf{u}$ and plastic deformation tensor $\mathbf{H}^p$, by

$$\mathrm{div}(\mathcal{E}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^p)) = 0, \quad \boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\mathrm{T}}\right), \quad \boldsymbol{\varepsilon}^p = \{\mathbf{H}^p\}^S. \quad (10)$$

The incremental equilibrium equation is obtain by deriving the above relation with respect to time and takes the form

$$\mathrm{div}\left(\mathcal{E}\left(\frac{1}{2}(\nabla\mathbf{v}+(\nabla\mathbf{v})^{\mathrm{T}}) - \{\dot{\mathbf{H}}^p\}^S\right)\right) = 0. \quad (11)$$

The evolution equation for the plastic distortion $\mathbf{H}^p$ is obtained from (7) and is given by

$$\xi_1\dot{\mathbf{H}}^p = -\beta_2\mathrm{curl}(\mathrm{curl}\mathbf{H}^p) + \mathbf{T}. \quad (12)$$

In order to obtain a boundary value problem we attach the boundary condition for the incremental equilibrium equation and for the evolution equation for the plastic distortion. Let Ω be the domain occupied by the body $\mathcal{B}$ at the moment t and $\Gamma = \partial\Omega$ be the boundary of Ω. We assume the following boundary conditions for the incremental equilibrium equation:

$$\dot{\mathbf{T}}\mathbf{n} = \dot{\mathbf{t}} \quad \text{on} \quad \Gamma_1, \quad \mathbf{v} = \mathbf{v}^* \quad \text{on} \quad \Gamma_2, \quad (13)$$

where $\Gamma_1 \cup \Gamma_2 = \Gamma$ and $\Gamma_1 \cap \Gamma_2 = \varnothing$, and for the evolution equation for the plastic distortion:

$$\boldsymbol{\alpha}(\boldsymbol{\varepsilon}\mathbf{n}) = (\mathrm{curl}\mathbf{H}^p)(\boldsymbol{\varepsilon}\mathbf{n}) = \mathbf{h}^p \quad \text{on} \quad \Gamma, \quad (14)$$

where $\mathbf{n}$ is the outward normal to the boundary of the domain Ω and ε represent Ricci permutation tensor.

5. THE WEAK FORMULATION IN THE CASE OF SMALL DISTORTIONS

The corresponding variational equality for the incremental equilibrium equation is given by:

$$\int_{\Omega}\left[\mathcal{E}\left(\frac{1}{2}(\nabla\mathbf{v}+(\nabla\mathbf{v})^{\mathrm{T}})-\{\dot{\mathbf{H}}^{p}\}^{S}\right)\right]\cdot\{\nabla\mathbf{w}\}^{S}\,\mathrm{d}\mathbf{x}-\int_{\Gamma_1}\dot{\mathbf{t}}\cdot\mathbf{w}\,\mathrm{d}A=0,\quad\forall\mathbf{w}\in\mathcal{V}_{ad}^{0}. \tag{15}$$

The unknown $\mathbf{v}\in\mathcal{V}_{ad}=\left\{\mathbf{v}:\Omega\to\mathbf{R}^{3}\mid\mathbf{v}=\mathbf{v}^{*}\text{ on }\Gamma_2\right\}$ and $\mathcal{V}_{ad}^{0}=\left\{\mathbf{w}:\Omega\to\mathbf{R}^{3}\mid\mathbf{w}=\mathbf{0}\text{ on }\Gamma_2\right\}$.

The weak form of the evolution equation for the plastic distortion can be characterized for any field $\mathbf{G}$

$$\int_{\Omega}\xi_1\dot{\mathbf{H}}^{p}\cdot\mathbf{G}\mathrm{d}\mathbf{x}=-\int_{\Omega}\beta_2\,(\,\mathrm{curl}\mathbf{H}^{p})\cdot(\mathrm{curl}\mathbf{G})\mathrm{d}\mathbf{x}+\beta_2\int_{\partial\Omega}\mathbf{h}^{p}\cdot\mathbf{G}\mathrm{d}A+\int_{\Omega}\mathbf{T}\cdot\mathbf{G}\mathrm{d}\mathbf{x}. \tag{16}$$

5.1. The discretization of the weak form for the evolution equations

Let us consider $(t_n)_{1\le n\le N}$ a partition of the time interval $[0,T]$ and $\mathrm{d}t=t_{n+1}-t_n$ be the increment of time. Let Ω^{n} be the domain occupied by the body on the $[t_n,t_{n+1}]$ interval. For the discretization we apply an implicit procedure. The time derivative of the plastic distortion is approximate by the formulae $\dot{\mathbf{H}}^{p}\approx\dfrac{\mathbf{H}_{n+1}^{p}-\mathbf{H}_{n}^{p}}{\mathrm{d}t}$ and the plastic distortion we approximate by $\mathbf{H}^{p}\approx\mathbf{H}_{n+1}^{p}$. With these considerations (in the $\mathbf{h}^{p}=0$ hypotheses) the discretization of the weak form for the plastic distortion becomes:

$$\int_{\Omega_n}\xi_1\frac{\mathbf{H}_{n+1}^{p}-\mathbf{H}_{n}^{p}}{\mathrm{d}t}\cdot\mathbf{G}\mathrm{d}\mathbf{x}=-\int_{\Omega_n}\beta_2\,(\,\mathrm{curl}\mathbf{H}_{n+1}^{p})\cdot(\mathrm{curl}\mathbf{G})\mathrm{d}\mathbf{x}+\int_{\Omega_n}\mathbf{T}_n\cdot\mathbf{G}\mathrm{d}\mathbf{x}. \tag{17}$$

5.2. The discretization of the weak form for the incremental equilbrium equation type

In the same way we obtain the discretization for the variational equality (15):

$$\int_{\Omega_n}\left[\mathcal{E}\left(\frac{1}{2}(\nabla\mathbf{v}_n+(\nabla\mathbf{v}_n)^{\mathrm{T}})-\left\{\frac{\mathbf{H}_{n+1}^{p}-\mathbf{H}_{n}^{p}}{dt}\right\}^{S}\right)\right]\cdot\{\nabla\mathbf{w}\}^{S}\,\mathrm{d}\mathbf{x}-\int_{\Gamma_n^{1}}\frac{\mathbf{t}_{n+1}-\mathbf{t}_{n}}{dt}\cdot\mathbf{w}\mathrm{d}A=0\,. \tag{18}$$

6. EDGE DISLOCATIONS

An *edge dislocation* is characterized by the components of the plastic distortion which generates a Burgers vector in the plane $(\mathbf{e}_1,\mathbf{e}_2)$, i.e. $\mathbf{b}\perp\mathbf{e}_3\Rightarrow\mathbf{b}=b_1\mathbf{e}_1+b_2\mathbf{e}_2$. The plastic distortion is given by: $\mathbf{H}^{p}=H_{11}^{(p)}\mathbf{e}_1\otimes\mathbf{e}_1+H_{12}^{(p)}\mathbf{e}_1\otimes\mathbf{e}_2+H_{21}^{p}\mathbf{e}_2\otimes\mathbf{e}_1+H_{22}^{(p)}\mathbf{e}_2\otimes\mathbf{e}_2$, where $H_{ij}^{(p)}=H_{ij}^{(p)}\left(x^1,x^2\right),\ i,j\in\{1,2\}$. The dislocation tensor takes the following form: $\boldsymbol{\alpha}=\mathrm{curl}\mathbf{H}^{p}=(\dfrac{\partial H_{12}^{(p)}}{\partial x^1}-\dfrac{\partial H_{11}^{(p)}}{\partial x^2})\mathbf{e}_1\otimes\mathbf{e}_3+(\dfrac{\partial H_{22}^{(p)}}{\partial x^1}-\dfrac{\partial H_{21}^{(p)}}{\partial x^2})\mathbf{e}_2\otimes\mathbf{e}_3$.

In our example it is assumed that the initial existing defects inside the microstructure are reduced to an area of dislocations, which is characterized by the dislocation tensor $\boldsymbol{\alpha}^{0}(\mathbf{x})$.

To find the initial condition for $\mathbf{H}^{p}(\mathbf{x})$, i.e. $\mathbf{H}_{0}^{p}(\mathbf{x})$, we follow the procedure proposed by [1] and [18]:

$$\left(\mathrm{curl}\mathbf{H}_0^{p}\right)\mathbf{e}_3=\mathbf{b}_0,\quad\mathrm{div}\mathbf{H}_0^{p}=0,\quad\forall\mathbf{x}\in\Omega,\quad\mathbf{H}_0^{p}=\mathbf{0},\quad\forall\mathbf{x}\in\partial\Omega. \tag{19}$$

This means that the following **problems** has to be satisfied by $H_{ij}^{(p)},\ i,j\in\{1,2\}$, respectively

$$H^p_{11,11}+H^p_{11,22}=-b^0_{1,2}\ \ \forall\mathbf{x}\in\Omega,\ \ H^p_{11}=0,\ \forall\mathbf{x}\in\partial\Omega;\ \ H^p_{12,11}+H^p_{12,22}=b^0_{1,1}\ \ \forall\mathbf{x}\in\Omega,\ \ H^p_{12}=0,\ \ \forall\mathbf{x}\in\partial\Omega;$$
$$H^p_{21,11}+H^p_{21,22}=-b^0_{2,2}\ \ \forall\mathbf{x}\in\Omega,\ \ H^p_{21}=0,\ \forall\mathbf{x}\in\partial\Omega;\ \ H^p_{22,11}+H^p_{22,22}=b^0_{2,1}\ \forall\mathbf{x}\in\Omega,\ \ H^p_{22}=0,\ \forall\mathbf{x}\in\partial\Omega. \quad (20)$$

We consider a distribution of Burger vectors parallel to the Ox_1 axis, i.e. $\mathbf{b}_0=b^0_1\mathbf{e}_1$. In the numerical simulation the function b^0_1 is defined by $b_1(t_0)=b_{max}\exp[-k(\frac{(x_1-x_0^{sup})^2}{a_x^2}+\frac{(x_2-y_0^{sup})^2}{a_y^2})],\quad (x_1,x_2)\in\Omega.$

The **algorithm** for solving the system of the equations (20), (15) and (16):

- The elastic problem is resolved until the averaged value of the equivalent stress state becomes equal or larger than a critical value, i.e. $\int_\Omega \sqrt{\mathbf{T}'\cdot\mathbf{T}'}\mathrm{d}\mathbf{x}/A(\Omega)<\sqrt{2/3}\sigma_y$. Assume that at time t_0 the stress reached the yield condition. We mention that $A(\Omega)$ represent the area of the domain Ω.
- At this moment we solve problems (20) by employing the finite element method (FEM). The fields $H^{(p)}_{ij}(t_0)$, represent the initial conditions for the evolution equation (12).
- For $t_n\ge t_0$
  - ✓ We suppose that at the moment t_n one knows the current state of the body, namely: $\mathbf{H}^p_n,\mathbf{v}_n$. By an implicit procedure we find the solutions for $\mathbf{H}^p$ at the moment of time t_{n+1}, namely $\mathbf{H}^p_{n+1}$;
  - ✓ We return at the discretisation of the weak form for equilibrium equation for the rate of displacement $\mathbf{v}$ and we find the solution at the moment of time t_{n+1}, namely $\mathbf{v}_{n+1}$.
  - ✓ One can update the mesh and all the measures calculated on the previous mesh, knowing the velocity field $\mathbf{v}_{n+1}$. The procedure continues.

In the numerical simulations, a bidimensional domain represented in Fig. 1, occupied by an aluminum crystal has been considered. In the tensile test, the edge $x_1=0$ (left side) is fixed. The numerical algorithms were performed using the FreeFem++ package [16]. The edge $x_1=L_0$ (right side) is moved with a constant speed $v_1=5.0\times10^{-2}\,\mathrm{nm}/\mu\mathrm{s}$ applied along the axis Ox_1 and is fixed along the axis Ox_2. The time integration step (time increment) $\mathrm{d}t=10^{-2}\mu\mathrm{s}$ generates an incremental elongation $\mathrm{d}\varepsilon_{11}=1.5\cdot10^{-5}$. The initial dimensions of the sheet are: total length $L_0=32$ nm, the maximum width $l_0^{ext}=6.5$ nm and the minimum width $l_0^{int}=5$ nm.

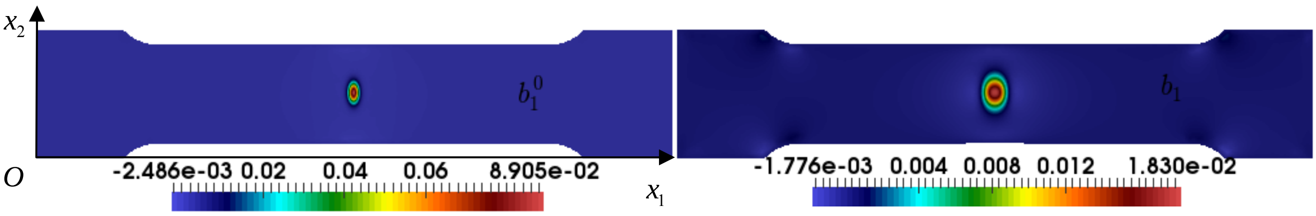
The values of the *material parameters* for aluminum [12]: $\mu=27\cdot10^3\,$MPa, $\nu=0.3$, $\sigma_y=70$MPa, $E_{1111}=E_{2222}=\frac{2\mu(1-\nu)}{1-2\nu}$, $E_{1122}=E_{2211}=\frac{2\mu\nu}{1-2\nu}$, $E_{1221}=E_{1212}=E_{2112}=E_{2121}=\mu$. The parameters appearing in the evolution equations are numerically evaluated in [10]: $\xi_1=5.7\cdot10^5\mu$sMpa, $\beta_2=5.7\cdot10^3\,$nm^{2}MPa. The *geometrical parameters* which characterize the initial values of the dislocations area are: $a_x=0.5$ nm, $a_y=1$nm, $x_0=L_0/2$nm, $y_0=l_0/2$nm, $k=4.6$.

In Fig.1 the initial inhomogeneity, represented by the dislocation tensor component $b_1=(\mathrm{curl}\mathbf{H}^p)_{13}$ is plotted at the moment when the plastic deformation is initialized (Fig. 1a) and at the total tensile strain of 1% (Fig. 1b). In the center of the sheet we observe the diffusion effect, as the defects are spreading, with an increase of the tensile strain. In Fig. 2 are represented the solution of the problems (20), i.e. the distribution of the plastic distortion tensor: $H^p_{11}(t_0)$ and $H^p_{12}(t_0)$, in the initial plastic state that corresponds to ε_{11}=0.1%.

The values of the equivalent deviatoric stress in the defect region are comparable with the values which appeared in the geometric concentration area (Fig. 3b). The elastic strain fields show dilatation and contraction in the defect zone (Fig. 4b) and shear along the vertical axis of the defect area (Fig. 4a).

In Fig. 3a, the equivalent plastic deformation is shown, and we remark the hardening of the material in the zone corresponding to the maximum value of $T^{ec}=\sqrt{\mathbf{T}'\cdot\mathbf{T}'}$ and the softening of the material in the zone corresponding to the minimum value of the equivalent deviatoric stress.

These numerical results are similar with the case in which is considered a dipole of disclinations only. In the paper [10] we emphasized that the Burgers vectors of the edge dislocations $(\alpha_{13}, \alpha_{23})$, which are inside the disclination dipole, is approximately normal to the dipole arm. This result is in agreement with the experiment [2]. The numerical test simulated in the present paper shows that a zone with normal Burgers vectors to the Ox_2 axis produce such effect similar to that of a dipole of disclinations with the axis in the Ox_2 direction.



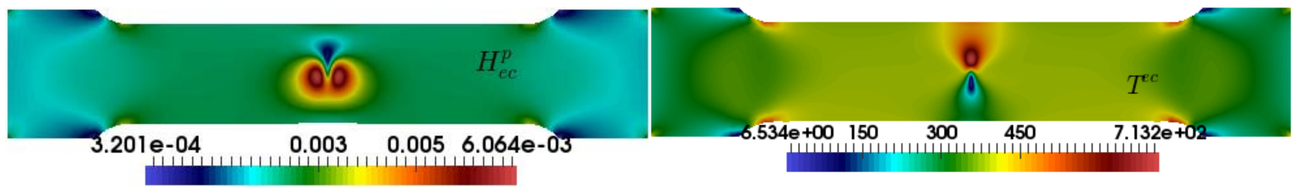
(a) (b)

Fig. 1 – Distribution of the dislocation tensor component $b_1 = \left(\text{curl}\mathbf{H}^p\right)_{13}$ in $\left[\text{nm}^{-1}\right]$:

a) in the initial plastic state that corresponds to ε_{11}=0.1% ; b) at the total tensile strain of 1%.

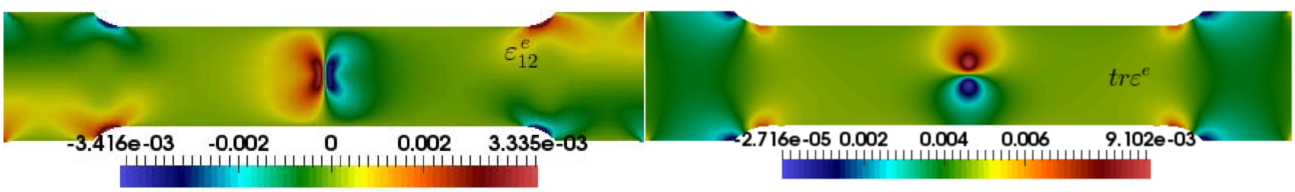
(a) (b)

Fig. 2 – Distribution of the plastic distortion tensor: a) $H_{11}^p\left(t_0\right)$; b) $H_{12}^p\left(t_0\right)$ in the initial plastic state.



(a) (b)

Fig. 3 – Distribution of: a) the equivalent plastic deformation $H_{ec}^p = \sqrt{\mathbf{H}^p \cdot \mathbf{H}^p}$; b) of the equivalent deviatoric stress $T^{ec} = \sqrt{\mathbf{T}' \cdot \mathbf{T}'}$ in MPa , at the total tensile strain of 1%.



(a) (b)

Fig. 4 – Distribution of: a) the elastic component ε_{12}^e ; b) of the $\text{tr}\boldsymbol{\varepsilon}^e$, at the total tensile strain of 1%.

CONCLUSIONS

The model describes the behaviour of crystalline materials with defects defined in terms of the incompatible plastic distortion. The model was proposed within the second order elasto-plasticity developed by Cleja-Tigoiu [4, 5, 8].The non-local *diffusion like evolution equation* for plastic distortion was derived to be compatible with the reduced dissipation inequality for *finite and small* deformation.

In order to validate the elasto-plastic model with edge dislocations, the initial and boundary value problem concerning the tensile test of a non-rectangular sheet was *solved numerically* in the hypothesis that, at the initial moment, a single area of dislocations describes the heterogeneity of defects.

The numerical results clearly showed the effects induced by the *initial heterogeneity.*

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