# Non-local elasto-viscoplastic models with dislocations

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We describe the behaviour of the elasto-plastic material:

• Based on the existence of configurations with torsion  $(\exists)\mathcal{K}_t \equiv \mathcal{K} \text{ config. with torsion } \iff$  $(\mathbf{F}^p, \overset{(p)}{\mathbf{\Gamma}}_k)$  plastic distorsion and plastic connection with torsion

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   (**F**<sup>p</sup>, Γ<sup>(p)</sup><sub>k</sub>) plastic distorsion and plastic connection with torsion
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- 2 Lattice defects consist of dislocations, described by the scalar density of dislocations  $\rho_{\mathcal{K}}^d$
- Free energy density function is postulated to be dependent on the scalar density of dislocations and of its gradient in  $\mathcal{K}$

$$\psi = \psi_{\mathcal{K}}(\mathbf{C}^{e}, \overset{(e)}{\mathcal{A}_{\mathcal{K}}}, (\mathbf{F}^{p})^{-1}, \overset{(p)}{\mathcal{A}_{\mathcal{K}}}, \rho_{\mathcal{K}}^{d}, \nabla_{\mathcal{K}}\rho_{\mathcal{K}}^{d})$$
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(1)

as a function dependent on

- the second order elastic deformation ( ${f C}^e, {{\cal A}_{\cal K}}^{(e)}$ )
- the plastic measure of deformation  $((\mathbf{F}^{p})^{-1}, \overset{(\mathrm{p})}{\mathcal{A}_{\mathcal{K}}})$
- $\bullet$  the scalar density of dislocation  $\rho_{\mathcal{K}}^d$  and its gradient

## Imbalanced free energy

Ax. The virtual internal power in  ${\cal K}$ 

$$\begin{aligned} \operatorname{virt}(\mathcal{P}_{\operatorname{int}})_{\mathcal{K}} &= \frac{1}{\rho} (\mathbf{T} + \mathbf{T}^{*}) \cdot \widetilde{\mathbf{L}}^{e} + \frac{1}{\rho_{\mathcal{K}}} \boldsymbol{\mu}_{\mathcal{K}} \cdot \operatorname{virt} \mathcal{L}_{\mathbf{L}^{p}}[\overset{(e)}{\mathcal{A}_{\mathcal{K}}}] + \\ &+ \frac{1}{\rho_{\mathcal{K}}} \boldsymbol{\Upsilon}_{\mathcal{K}}^{p} \cdot \widetilde{\mathbf{L}}^{p} + \frac{1}{\rho_{\mathcal{K}}} \boldsymbol{\mu}_{\mathcal{K}}^{p} \cdot \nabla_{\mathcal{K}} \widetilde{\mathbf{L}}^{p} + \frac{1}{\rho_{\mathcal{K}}} \boldsymbol{\Upsilon}_{\mathcal{K}}^{\lambda} \cdot (\delta \mathbf{\Lambda}) + \\ &+ \frac{1}{\rho_{\mathcal{K}}} \boldsymbol{\Upsilon}_{\mathcal{K}}^{d} \cdot \delta \rho_{\mathcal{K}}^{d} + \frac{1}{\rho_{\mathcal{K}}} \boldsymbol{\mu}_{\mathcal{K}}^{d} \cdot \nabla_{\mathcal{K}} \delta \rho_{\mathcal{K}}^{d}. \end{aligned}$$

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**Ax.** The elasto-plastic behavior of the material is restricted to satisfy in  $\mathcal{K}$  the imbalanced free energy condition

 $-\dot{\psi}_{\mathcal{K}} + (\mathcal{P}_{int})_{\mathcal{K}} \ge 0$  for any virtual (isothermic) processes. (2)

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Micro stress and stress momentum

• obey the balance equations for micro forces:

$$\Upsilon^{p}_{\mathcal{K}} = {\sf div}\;(\mu^{p}_{\mathcal{K}} - \mu_{\mathcal{K}}) + \widetilde{
ho}B^{p}_{m}, \quad {\sf in}\; \mathcal{K}(\mathcal{P},t), \quad {\sf plastic \ micro \ forces}$$

 $\Upsilon^d_{\mathcal{K}} = {\rm div}_{\mathcal{K}} \; \mu^d_{\mathcal{K}} + \tilde{\rho} B^d_m, \quad \text{associated with the scalar dislocations}$ 

• satisfy the viscoplastic type constitutive equations

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#### Thermomechanics restrictions

#### are derived from the energy imbalance:

- Elastic type constitutive equations
- Evolution equations for  $\mathcal{K}_t$  have to be compatible with the dissipation inequlity.

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## Model with couple stresses and plastic connection:

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- S. C-T., Int.J. Fracture (2010)
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- The paper deals with a special case of elasto-plastic models within the crystal plasticity framework, i.e. no gradient of plastic distorsion is involved.
- The behaviour of the material is linear elastic with respect to plastically deformed configuration, without macro stress momnetum.
- The complet set of evolution equations has been derived, following Bortoloni and Cermelli (2004).
- The initial and boundary value problem for elasto-vascoplastic model with non-local equation for the scaler dislocation densities has been derived.

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- The complet set of evolution equations has been derived, following Bortoloni and Cermelli (2004).
- The initial and boundary value problem for elasto-vascoplastic model with non-local equation for the scaler dislocation densities has been derived.
- As applications in the paper by Bortoloni and Cermelli (2004):
  - the elastic behaviour is neglected
  - the shear stress is kept constant.
  - only one slip system is activated.

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## Elastic response

- Stress measures: T Cauchy
- S- first Piola-Kirchhoff in ref. config.
- **Π**− second Piola-Kirchhoff in relax. config.

 $\tilde{
ho}, \hat{
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## Elastic response

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 $\tilde{\rho}, \hat{\rho} ~\tilde{\rho}_{\rm 0} -$  mass densities.

• elastic type constitutive equation (if  $\exists$  the potential  $\varphi$ .)

$$\mathbf{\Pi} = \tilde{\rho} \frac{\partial \varphi(\mathbf{E}^e)}{\partial \mathbf{E}^e}, \qquad \mathbf{E}^e = \frac{1}{2} (\mathbf{F}^{e\,T} \mathbf{F}^e - \mathbf{I}) \quad \text{relax. config.}$$

$$\mathsf{T} = \hat{
ho} \mathsf{F}^e rac{\partial arphi(\mathsf{E}^e)}{\partial \mathsf{E}^e} (\mathsf{F}^e)^{\mathcal{T}} \quad \mathsf{def. \ config.}$$

$$\mathbf{S} = \hat{\rho}_0 \ \mathbf{F}^e \frac{\partial \varphi(\mathbf{E}^e)}{\partial \mathbf{E}^e} (\mathbf{F}^p)^{-T}, \qquad \text{ref. config.}$$

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#### • linear momentum balance equation

$$div \mathbf{T} = 0 \quad \text{in} \quad \chi(\mathcal{B}, t)$$

$$div \mathbf{S} = 0 \quad \text{in} \quad \mathcal{B}$$
(6)

when the boby forces are neglected.

• angular momentum balance equation

$$\mathbf{T} = \mathbf{T}^T \quad \Longleftrightarrow \quad \mathbf{F}\mathbf{S}^T = \mathbf{S}\mathbf{F}^T \tag{7}$$

## Rate of plastic distortion

evolution equation for the plastic distortion

$$\dot{\mathsf{F}}^{p}(\mathsf{F}^{p})^{-1} = \sum_{\alpha=1}^{N} \nu^{\alpha} \bar{\mathbf{s}}^{\alpha} \otimes \bar{\mathbf{m}}^{\alpha}$$
(8)

with N- the number of the slip-systems,  $(\mathbf{\bar{s}}^{\alpha}, \mathbf{\bar{m}}^{\alpha})$  the  $\alpha$ - slip system,  $\mathbf{\bar{m}}^{\alpha}$ - normal to the slip plane,  $\mathbf{\bar{s}}^{\alpha}$ - and  $\mathbf{\bar{s}}^{\alpha} \cdot \mathbf{\bar{m}}^{\alpha} = 0$ .  $\nu^{\alpha} = \dot{\gamma}^{\alpha}$ - slip velocity  $\gamma^{\alpha}$ - plastic shear on  $\alpha$ - slip system.

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## Rate of plastic distortion

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 $\nu^{\alpha} = \dot{\gamma}^{\alpha}$ - slip velocity  
 $\gamma^{\alpha}$ - plastic shear on  $\alpha$ - slip system.

•  $(\bar{\mathbf{s}}^{\alpha}, \bar{\mathbf{m}}^{\alpha})$  of the  $\alpha$ - slip system are considered to be fixed with respect to the reference configuration (see Mandel (1971) and Teodosiu (1976))

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## viscoplastic flow

• is described by:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_{0} \left| \frac{\tau^{\alpha}}{\zeta^{\alpha}} \right|^{n} \operatorname{sgn} \tau^{\alpha} H(\mathcal{F}^{\alpha}), \quad \nu^{\alpha} \equiv \dot{\gamma}^{\alpha} \quad \forall \alpha = 1, \dots, N,$$
(9)

 $H(\mathcal{F}^{lpha})$  is the Heaviside function composed with

• the activation function  $\mathcal{F}^{lpha}$ 

$$\mathcal{F}^{\alpha} := |\tau^{\alpha}| - \zeta^{\alpha} \tag{10}$$

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 $au^{lpha}-$  resolved shear stress  $\zeta^{lpha}-$  yield modulus (critical shear stress).

via the Schmid's law

$$|\tau^{\alpha}| \ge \zeta^{\alpha} \Leftrightarrow \mathcal{F}^{\alpha} := |\tau^{\alpha}| - \zeta^{\alpha} \ge 0$$
 (11)

### resolved shear stress

 $\bullet\,$  is defined in terms of  ${\bf T}$  or  ${\bf S}\,$ 

$$\tau^{\alpha} := \frac{\mathbf{T}}{\hat{\rho}} \mathbf{m}^{\alpha} \cdot \mathbf{s}^{\alpha}, \quad \mathbf{s}^{\alpha} = \mathbf{F}^{e} \mathbf{\bar{s}}^{\alpha}, \quad \mathbf{m}^{\alpha} = (\mathbf{F}^{e})^{-T} \mathbf{\bar{s}}^{\alpha},$$

$$\tau^{\alpha} = \frac{1}{\hat{\rho}_{0}} \left( \mathbf{S} (\mathbf{F}^{p})^{T} \mathbf{\bar{m}}^{\alpha} \right) \cdot \mathbf{F}^{e} \mathbf{\bar{s}}^{\alpha}.$$
(12)

• *hardening law* is expressed either in terms of the dislocation densities, Cermelli and Bortoloni (2004):

$$\zeta^{\alpha} = \zeta^{\alpha} \left( \rho^{\beta} \right), \ \beta = 1, \dots, N.$$
(13)

or by certain evolution equation, Teodosiu and Raphanel (1993)

$$\dot{\zeta}^{\alpha} = \sum_{\beta=1}^{N} h^{\alpha\beta} \left| \dot{\gamma}^{\beta} \right| \tag{14}$$

non-local evolution equation

• for the dislocation densities considered by Bortoloni and Cermelli (2004)

$$\dot{\rho}^{\alpha} = D \left| \nu^{\alpha} \right| \left( k \Delta \rho^{\alpha} - \frac{\partial \psi_{T}}{\partial \rho^{\alpha}} \right), \alpha = 1, \dots, N$$
 (15)

where

$$\psi_{\mathcal{T}} = \psi_{\mathcal{T}}\left(\rho^{\beta}\right), \beta = 1, \dots, N$$
 (16)

is a dislocation energy, D are k constant.

boundary conditions

$$k\frac{\partial\rho^{\alpha}}{\partial n} = i^{\alpha} \left(\rho^{\beta}\right) \text{ pe } \partial B^{p}(t)$$
 (17)

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Simple shear in stress controlled test, for only one slip system Elastic solution

# General problem

- F,  $\gamma^{\alpha}(i.e.F^{p})$ ,  $\rho^{\alpha}$ , for  $\alpha = 1, ..., N$  defined on  $B \times [0, T)$ ,
- equilibrium equation  $div \mathbf{S} = 0$
- elastic type constitutive equation

$$\mathbf{S} = \mathbf{F}(\mathbf{F}^{p})^{-1} \left[ \frac{1}{2} \lambda tr((\mathbf{F}^{p})^{-T} \mathbf{F}^{T} \mathbf{F}(\mathbf{F}^{p})^{-1} - \mathbf{I}) \mathbf{I} + \mu \left( (\mathbf{F}^{p})^{-T} \mathbf{F}^{T} \mathbf{F}(\mathbf{F}^{p})^{-1} - \mathbf{I} \right) (\mathbf{F}^{p})^{-T}$$
(18)

• Evolution equation for plastic distortion

$$\dot{\mathsf{F}}^{\rho} = \left[\sum_{\alpha=1}^{N} \left| \frac{\mathsf{S}(\mathsf{F}^{\rho})^{T} \bar{\mathbf{m}}^{\alpha} \cdot \mathsf{F}(\mathsf{F}^{\rho})^{-1} \bar{\mathbf{s}}^{\alpha}}{\zeta^{\alpha}(\rho^{\beta})} \right|^{n} H\left(\mathcal{F}^{\alpha}\right) \operatorname{sgn}(\tau^{\alpha}) \bar{\mathbf{s}}^{\alpha} \otimes \bar{\mathbf{m}}^{\alpha} \right] \mathsf{F}^{\rho}$$

• Evolution equations for the dislocation densities

$$\dot{\rho}^{\alpha} = D \left| \frac{\mathbf{S}(\mathbf{F}^{\rho})^{T} \mathbf{\tilde{m}}^{\alpha} \cdot \mathbf{F}(\mathbf{F}^{\rho})^{-1} \mathbf{\bar{s}}^{\alpha}}{\zeta^{\alpha}(\rho^{\beta})} \right|^{n} H(\mathcal{F}^{\alpha}) \left( k \Delta \rho^{\alpha} - \frac{\partial \psi_{T}}{\partial \rho^{\alpha}} \right), \ \alpha = 1, \dots, N$$

#### • Boundary conditions

$$\mathbf{Sn} = \overline{\mathbf{t}}^0 \text{ on } \Gamma_1^0$$
$$\mathbf{u} = \overline{\mathbf{u}} \text{ on } \Gamma_2^0$$
$$k \frac{\partial \rho^{\alpha}}{\partial n} = i^{\alpha} (\rho^{\beta}) \text{ on } \partial B^p(t)$$
(20)

• Initial conditions

$$\gamma^{\alpha}(0) = 0 \quad \rho^{\alpha}(0) = \rho_{0}^{\alpha} \quad \alpha = 1, \dots, N \quad \Longleftrightarrow \quad \mathbf{F}^{\rho}(0) = \mathbf{I}$$
(21)

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Simple shear in stress controlled test, for only one slip system  $\ensuremath{\mathsf{Elastic}}$  solution

## Statement of the problem



domain occupied by the body is a layer B

 $B = \{(x, y, z) : 0 \le z \le L\} \mapsto (\mathbb{D} \setminus (\mathbb{D} \setminus \mathbb{C})) \to (\mathbb{D} \setminus \mathbb{C})$ 

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Simple shear in stress controlled test, for only one slip system  $\ensuremath{\mathsf{Elastic}}$  solution

- Only one slip system ( ${\bf \bar{s}}\equiv {\bf i}, ~~{\bf \bar{m}}\equiv {\bf k},$
- plastic distortion

$$\mathbf{F}^{p} = \mathbf{I} + \gamma \mathbf{\bar{s}} \otimes \mathbf{\bar{m}}, \quad \dot{\gamma} = \nu \tag{23}$$

• Problem: For a given homogeneous shear stress state,

$$\mathbf{S} = S_{13}(t) \left( \mathbf{i} \otimes \mathbf{k} + \mathbf{k} \otimes \mathbf{i} 
ight)$$
 with  $S_{13} : [t_0, T) \longrightarrow R_{\geq 0}$ 

find the unknowns

$$\mathbf{F} = \mathbf{F}(z, t), \rho = \rho(z, t) \text{ si } \gamma = \gamma(z, t), \text{ defined on } B \times [t_0, T)$$

• Elastic type constutive equation

$$S_{13}(t) (\mathbf{i} \otimes \mathbf{k} + \mathbf{k} \otimes \mathbf{i}) =$$

$$= \mathbf{F} (\mathbf{I} + \gamma \mathbf{s} \otimes \mathbf{m})^{-1} \left[ \frac{1}{2} \lambda tr((\mathbf{I} + \gamma \mathbf{s} \otimes \mathbf{m})^{-T} \mathbf{F}^{T} \mathbf{F} (\mathbf{I} + \gamma \mathbf{s} \otimes \mathbf{m})^{-1} - \mathbf{I}) + \mu \left( (\mathbf{I} + \gamma \mathbf{s} \otimes \mathbf{m})^{-T} \mathbf{F}^{T} \mathbf{F} (\mathbf{I} + \gamma \mathbf{s} \otimes \mathbf{m})^{-1} - \mathbf{I} \right) \right] (\mathbf{I} + \gamma \mathbf{s} \otimes \mathbf{m})^{-T}$$

 $\bullet\,$  Evolution equation for  $\gamma$ 

$$\dot{\gamma} = \left| \frac{S_{13}(t)F_{11}}{\zeta(\rho)} \right|^n \operatorname{sgn}\left(S_{13}(t)F_{11}\right) H(|\tau| - \zeta(\rho))$$
(24)

• Evolution equation for the dislocation density

$$\dot{\rho} = D \left| \frac{S_{13}(t)F_{11}}{\zeta(\rho)} \right|^n \left( k\Delta\rho - \frac{\partial\psi\tau}{\partial\rho} \right) H(|\tau| - \zeta(\rho))$$
(25)

• Activation condition defined in terms of

$$|\tau| - \zeta(\rho) \equiv |S_{13}(t)F_{11}| - \zeta(\rho).$$
 (26)

Initial condition

$$\gamma(z,0) = 0, \quad \rho(z,0) = \rho_0(z)$$
 (27)

boundary conditions

$$\frac{\partial \rho}{\partial z}(0,t) = \frac{\partial \rho}{\partial z}(L,t) = 0$$
(28)

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• liniar elastic response

$$\mathbf{S} = \mathbf{F}(\mathbf{F}^{p})^{-1} \left(\lambda tr(\mathbf{E}^{e})\mathbf{I} + 2\mu \mathbf{E}^{e}\right) (\mathbf{F}^{p})^{-T}.$$
 (29)

• Solve the problem for

 $\mathbf{F}^{
ho}(t) = \mathbf{I}(i.e.\gamma(t) = 0), 
ho(t) = 
ho(0)$  on certain time interval [0, a

Simple shear in stress controlled test, for only one slip system Elastic solution

#### Theorem

$$\mathbf{F} = \begin{pmatrix} F_{11} & F_{12} & F_{13} \\ 0 & F_{22} & 0 \\ F_{13} & F_{32} & F_{11} \end{pmatrix}$$
(30)

with

$$F_{22} = \sqrt{F_{11}^2 + 3F_{13}^2}$$

$$F_{11} = \sqrt{\frac{S_{13}}{2\mu F_{13}} + F_{13}^2}, \quad if \quad F_{13} \neq 0,$$
(31)

and  $F_{13} = x$  solution of the equation

$$F_{13}^{3} - \frac{(3\lambda + 2\mu)}{8(\lambda + \mu)}F_{13} + S_{13}\frac{(3\lambda + 2\mu)}{16\mu(\lambda + \mu)} = 0$$
(32)

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#### Theorem

Solution of the equation for 
$$x = F_{13}$$

$$x^{3} + Ax + B = 0$$
  
with  $A = -\frac{(3\lambda + 2\mu)}{8(\lambda + \mu)}, \quad B = S_{13}\frac{(3\lambda + 2\mu)}{16\mu(\lambda + \mu)} \equiv \frac{S_{13}}{2\mu}A$  (33)

are given under the form

$$x_1 = -a - b$$

$$x_2 = \frac{a+b+\sqrt{-3(a-b)^2}}{2}, \quad x_3 = \frac{a+b-\sqrt{-3(a-b)^2}}{2}$$

where

$$b = \sqrt[3]{\frac{B - \sqrt{\Delta_t}}{2}}, \quad a = -\frac{A}{3\sqrt[3]{\frac{B + \sqrt{\Delta_t}}{2}}} \tag{35}$$

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The solutions of the algebraic equation for  $F_{13}$  can be characterized through the signum of the expression

$$\Delta_{t} = B^{2} + 4\left(\frac{A}{3}\right)^{3} \equiv \left\{\left(\frac{S_{13}}{2\mu}\right)^{2} - \frac{2(3\lambda + 2\mu)}{27(\lambda + \mu)}\right\} \left[\frac{3\lambda + 2\mu}{16(\lambda + \mu)}\right]^{2} (36)$$
$$\Delta_{t} \leq 0 \iff S_{13} \leq \mu \sqrt{\frac{2}{27} \frac{3\lambda + 2\mu}{\lambda + \mu}}$$

 $\iff$  three real solutions exist, but either all are diffrent

$$\Delta_t > 0 \iff S_{13} > \mu \sqrt{rac{2}{27} rac{3\lambda + 2\mu}{\lambda + \mu}}$$

 $\iff$  only one real and two complex cojugated solutions e (37)

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## Elastic solution



The three possible elastic solutions, for shear component of deformation  $F_{13}$ 

Elastic solution

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The non-zero components of the elstic solution

## Conclusions

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To solve the general problem:

• First we solve the elastic solution in order to determine the critical stress state at which the activation criterion is reached, see the detail in 2.2.

# Conclusions

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To solve the general problem:

- First we solve the elastic solution in order to determine the critical stress state at which the activation criterion is reached, see the detail in 2.2.
- Second we solve the sistem of equations, starting from the initial conditions that correspond to the critical stress state reached from the elastic solutions.

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# Conclusions

- 1. Graphics representations
  - for the plastic shear  $\gamma,$
  - the dislocation densities  $\rho$ , and the non-vanishing components of the deformation gradients,  $F_{13}, F_{31}, F_{11} = F_{33}, F_{22}$

have been ploted in a spatial representation, as functions of the time t and the position z of the material points in the layer.

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# Conclusions

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have been ploted in a spatial representation, as functions of the time t and the position z of the material points in the layer.
2. To develope a finite element description of the large deformation of a polycrystalline body (following Teodosiu, Raphanel -1993, Simo, Hughes-2000) for non-local models

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## Disclocation densities $\rho(t, z)$



The evolution of non-homogeneous dislocation density

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## Plastic shear $\gamma(t, z)$ )



The evolution of non-homogeneous plastic shear

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### Non-zero components of the deformation gradient



 $F_{11}$  – component of the deformation gradient

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## Non-zero components of the deformation gradient F(t,z)



 $F_{13}$  – component of the deformation gradient

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## Non-zero components of the deformation gradient F(t,z)



 $F_{22}$  – component of the deformation gradient

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## Non-zero components of the deformation gradient F(t,z)



 $F_{31}$  – component of the deformation gradient

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## Non-zero components of the deformation gradient F(t,z)



 $F_{33}$  – component of the deformation gradient

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# Non-zero components of the deformation gradient for z = 0.1205



#### All non-vanishing components of the deformation gradient

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Simple shear in stress controlled test, for only one slip system Elastic solution

# Non-zero components of the elastic distorsion for z = 0.1205



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