Computing polycrystalline aggregates for comparison with field measurements

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1. Microstructural mechanics
   - Morphology of polycrystalline aggregates
   - Continuum crystal plasticity
   - Validation of the continuum approach
2. Strain heterogeneities in bulk polycrystals
   - Representative volume element size
   - Hierarchy of heterogeneity levels in polycrystals
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5. Continuum modelling of size effects in polycrystals
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   - Grain size effect

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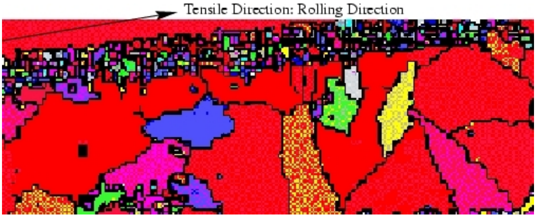
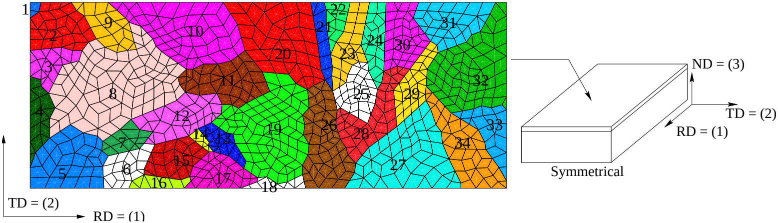
Characterization of thin layers and coatings

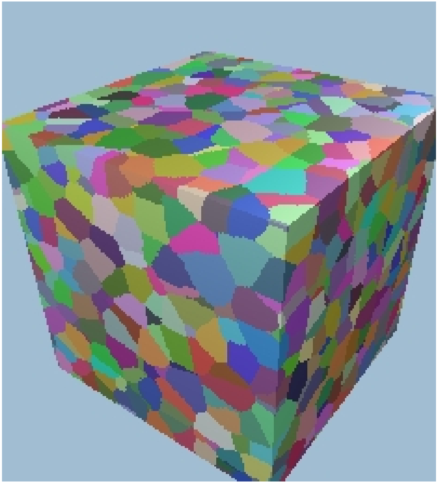


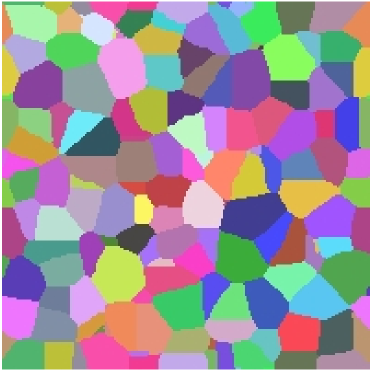
coating of a galvanized steel sheet
EBSD analysis



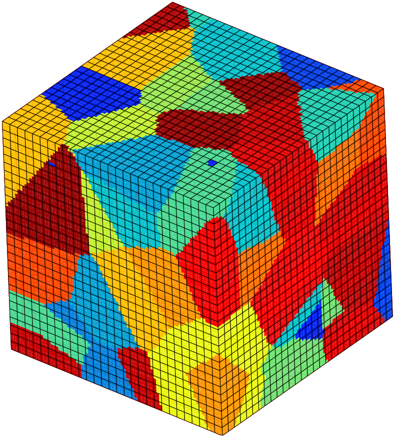
2D geometry but 3D deformation modes!

Models for polycrystals : Voronoi mosaics

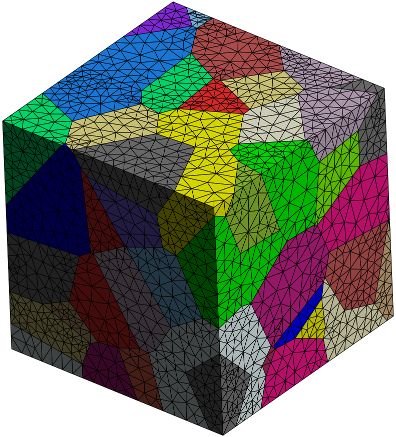




Meshing polycrystals : Voronoi cells

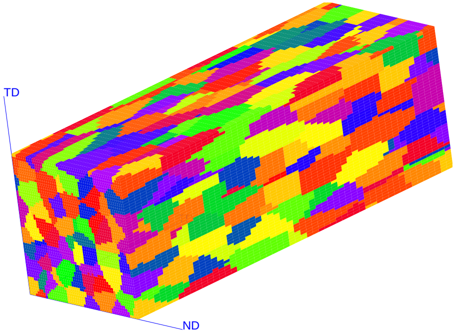


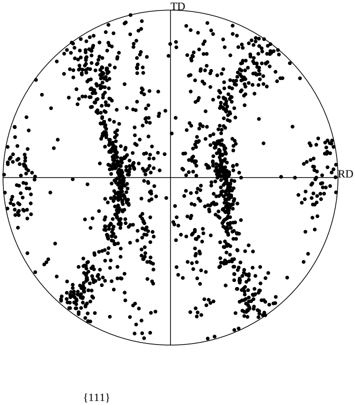
multiphase elements



free meshing

Morphological and crystallographic texture





cupro–beryllium alloy

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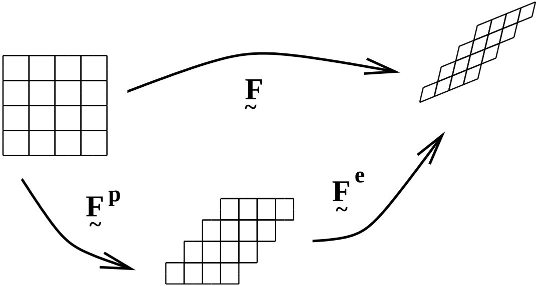
Continuum crystal plasticity theory

multiplicative decomposition [Mandel, 1973]

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{F}}^e . \underset{\sim}{\mathbf{F}}^p,$$

$$\dot{\underset{\sim}{\mathbf{F}}}^p . \underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s=1}^{n} \dot{\gamma}^s \underset{\sim}{\mathbf{P}}^s$$

$$\underset{\sim}{\mathbf{P}}^s = \underline{\mathbf{m}}^{\,s} \otimes \underline{\mathbf{n}}^{\,s}$$



Schmid law and viscoplastic flow

$\tau^s = \underset{\sim}{\mathbf{P}}^s : \underset{\sim}{\boldsymbol{\sigma}}$

$\dot{\gamma}^s = < \frac{|\tau^s - x_s| - r^s}{k} >^n \operatorname{sign} \tau^s$

isotropic hardening $\qquad r^s = r_0 + q \sum_{r=1}^{n} h^{sr} (1 - \exp(-b v^r))$

kinematic hardening $\qquad x^s = c^s \alpha^s, \quad \dot{\alpha}^s = \dot{\gamma}^s - d|\dot{\gamma}^s|\alpha^s$

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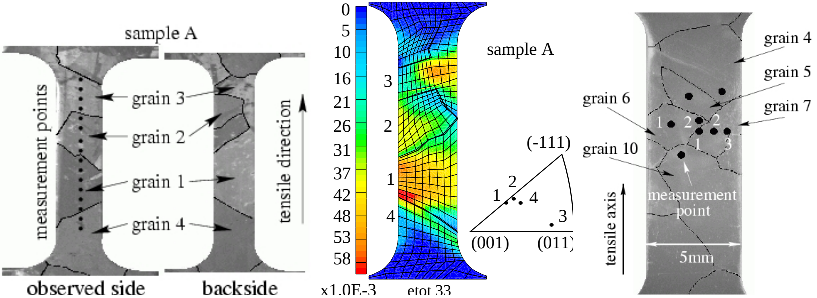
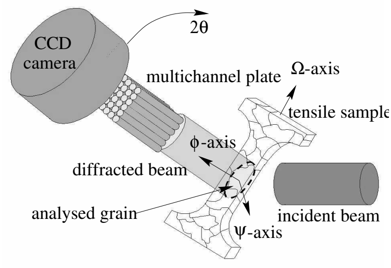
Multi–crystalline specimens



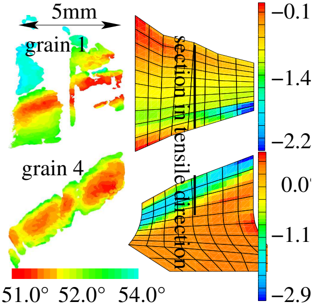
[Eberl, 2002]

Comparison with topographical X–ray diffraction measurements

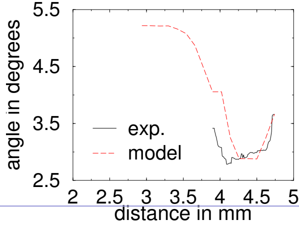


G3-beamline HASYLAB
elastic strain tensor field

[Eberl, 2002]



lattice rotation map



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Boundary conditions for material volume elements

- **Kinematic uniform boundary conditions (KUBC)** :

$$\underline{\mathbf{u}} = \underset{\sim}{\mathbf{E}}.\underline{\mathbf{x}} \quad \forall \underline{\mathbf{x}} \in \partial V$$

$$< \underset{\sim}{\varepsilon} >= \frac{1}{V}\int_V \underset{\sim}{\varepsilon}\, dV = \underset{\sim}{\mathbf{E}} \quad and \quad \underset{\sim}{\mathbf{\Sigma}} \hat{=} < \underset{\sim}{\sigma} >= \frac{1}{V}\int_V \underset{\sim}{\sigma}\, dV$$

- **Static uniform boundary conditions (SUBC)** :

$$\underset{\sim}{\sigma}.\underline{\mathbf{n}} = \underset{\sim}{\mathbf{\Sigma}}.\underline{\mathbf{n}} \quad \forall \underline{\mathbf{x}} \in \partial V$$

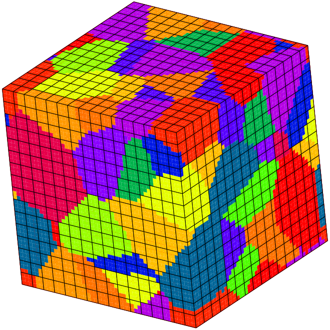
$$< \underset{\sim}{\sigma} >= \frac{1}{V}\int_V \underset{\sim}{\sigma}\, dV = \underset{\sim}{\mathbf{\Sigma}} \quad and \quad \underset{\sim}{\mathbf{E}} \hat{=} < \underset{\sim}{\varepsilon} >= \frac{1}{V}\int_V \underset{\sim}{\varepsilon}\, dV$$

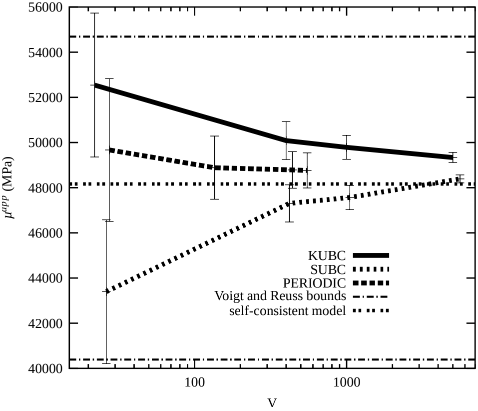
- **Periodicity conditions (PERIODIC)** :

$$\underline{\mathbf{u}} = \underset{\sim}{\mathbf{E}}.\underline{\mathbf{x}} + \underline{\mathbf{v}} \quad \forall \underline{\mathbf{x}} \in V,\ \underline{\mathbf{v}}\ \ periodic$$

RVE for elastic copper crystals

isotropic texture





$$C_{11} = 168400 \text{ MPa}, \quad C_{12} = 121400 \text{ MPa}, \quad C_{44} = 75390 \text{ MPa}$$

cubic elasticity $a = 2C_{44}/(C_{11} - C_{12}) = 3.2$

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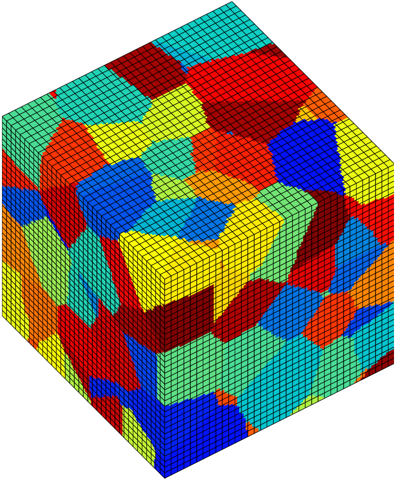
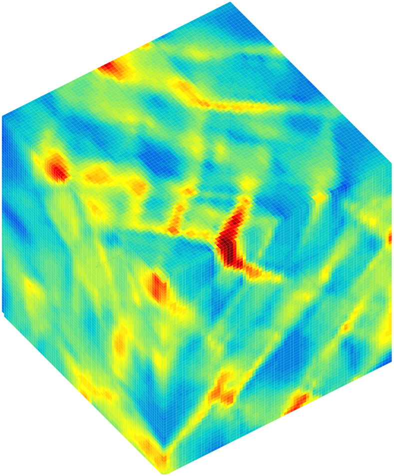
Elastoplastic deformation of polycrystalline aggregates

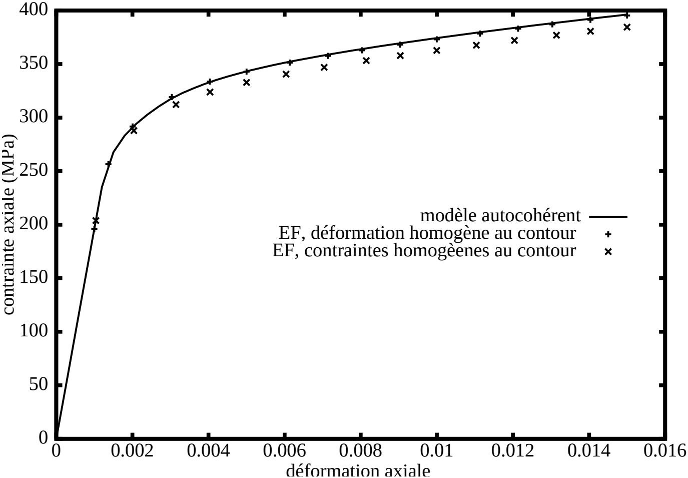


RVE for the polycrystal

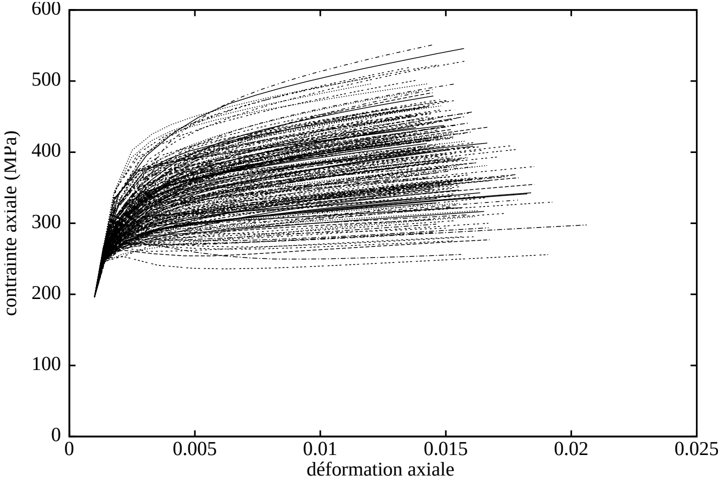


cumulative plastic strain

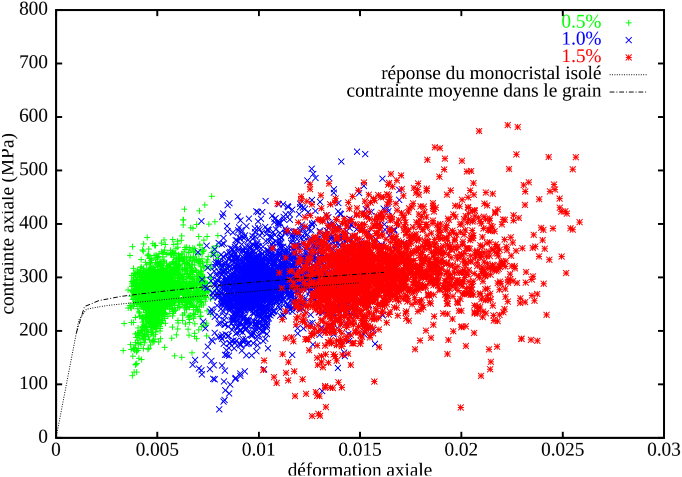
Macroscopic response



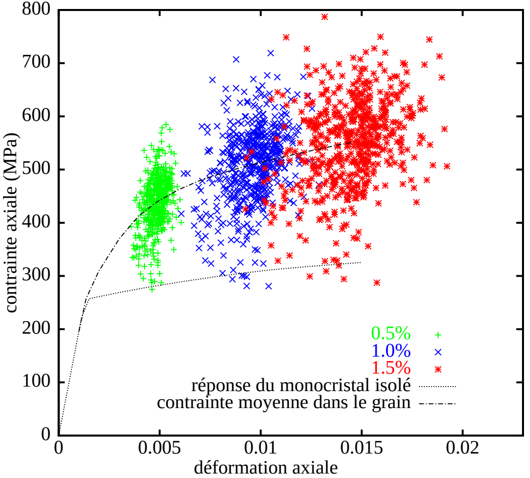
Mean response per grain



Local response in one grain



Local response in one grain



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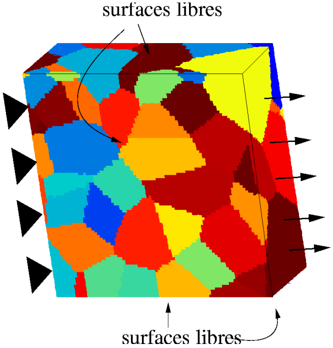
Boundary value problem



Copper (FCC)

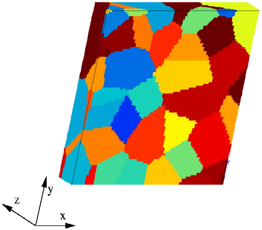
- anisotropic elasticity

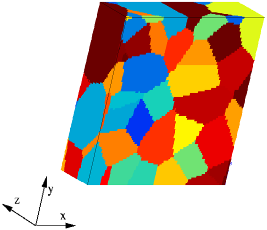
  $$C_{11} = 159300 \text{ (MPa)}$$
  $$C_{12} = 122000 \text{ (MPa)}$$
  $$C_{44} = 81000 \text{ (MPa)}$$

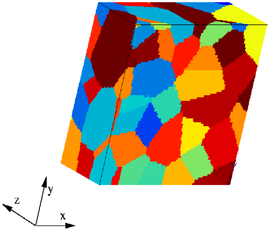
  anisotropy coefficient
  $a = 4.34$

- continuum crystal plasticity [Méric, Gaspérini, Cailletaud 1994]

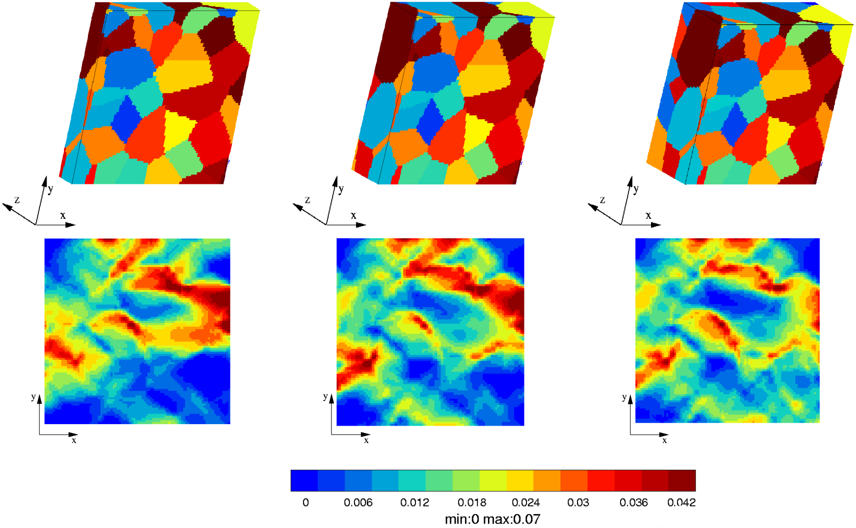
Range of plastic deformation







Range of plastic deformation



cumulative amount of slip : $\gamma_{eq} = \sum_{s=1}^{12} |\gamma|$ for $E_{22} = 1$ %

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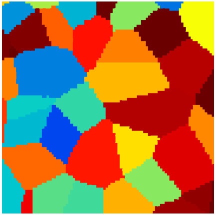
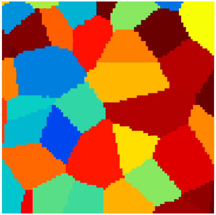
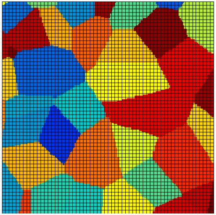
What is the grain morphology below a given surface ?



given surface grain morphology

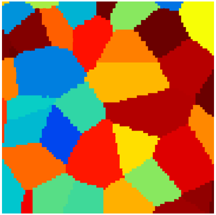
What is the grain morphology below a given surface ?



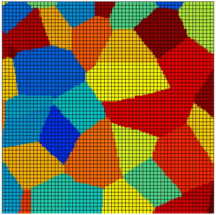


given surface grain morphology associated FE mesh

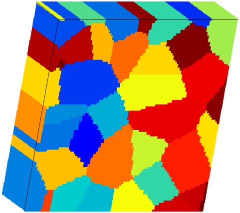
What is the grain morphology below a given surface ?



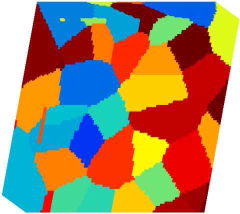
given surface grain morphology



associated FE mesh

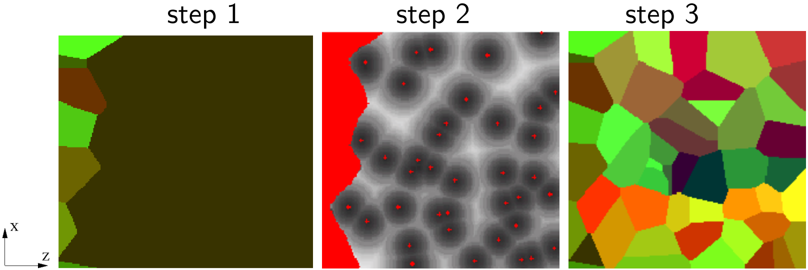


columnar grains



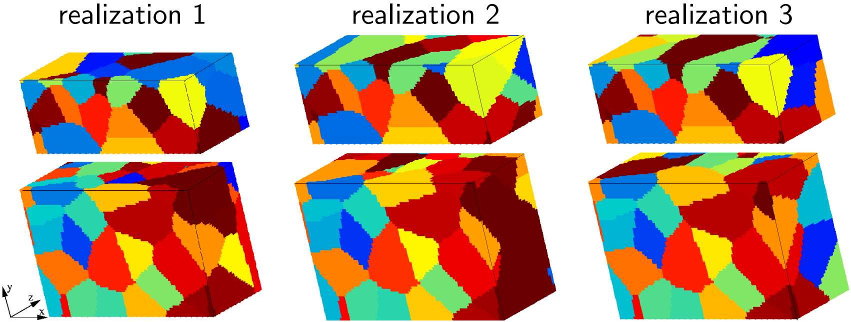
Voronoi polyhedra

Construction of 3D aggregates with prescribed surface morphology



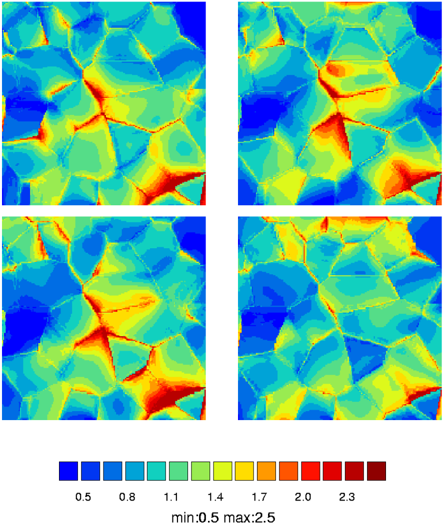
[N'Guyen, 2005]

Construction of 3D aggregates with prescribed surface morphology

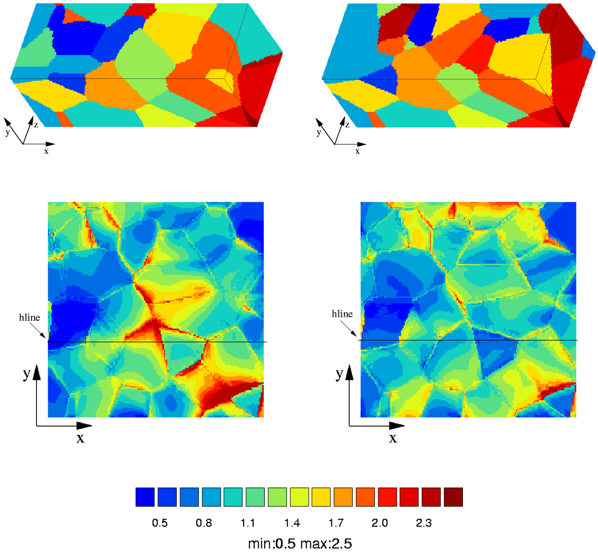


von Mises equivalent stress field

$\sigma_{eq}(\underline{\mathbf{x}})/\Sigma_{eq}$



Comparison between realizations 1 and 2



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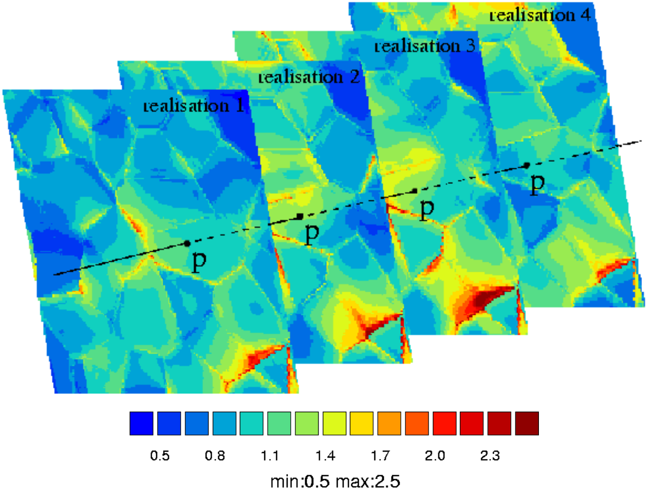
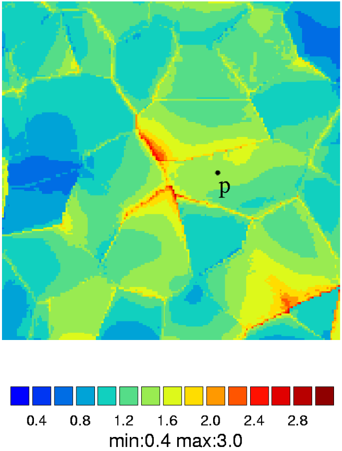
Surface ensemble averaging

Ensemble average: $\overline{\sigma}_{eq}(P) = \dfrac{1}{17} \displaystyle\sum_{i=1}^{17} \sigma^i_{eq}(P)$



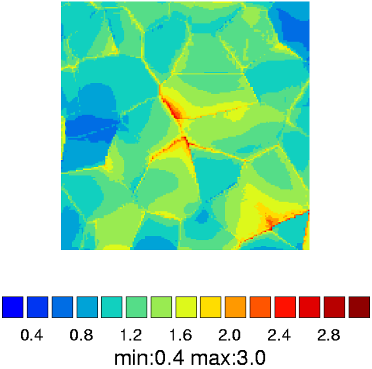
Ensemble average field for anisotropic elasticity

$\bar{\sigma}_{eq}(P)/\bar{\Sigma}_{eq}$

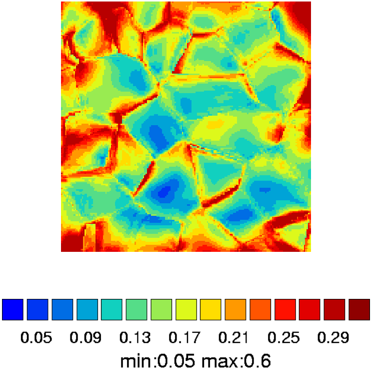


Ensemble average and relative variance for anisotropic elasticity

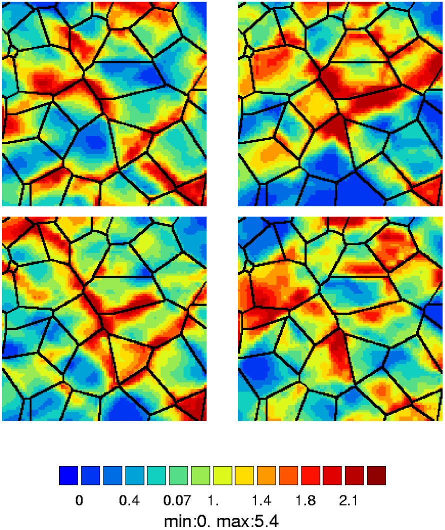
$\bar{\sigma}_{eq}/\bar{\Sigma}_{22}$



$D(\sigma_{eq})/\bar{\sigma}_{eq}$



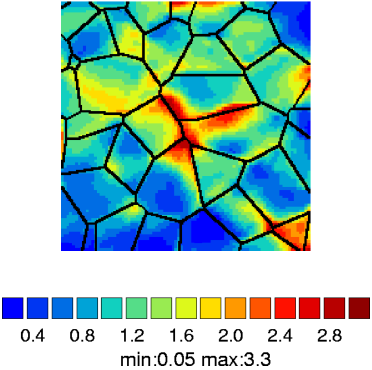
Plastic strain field for a tensile test $E_{22} = 2\%$



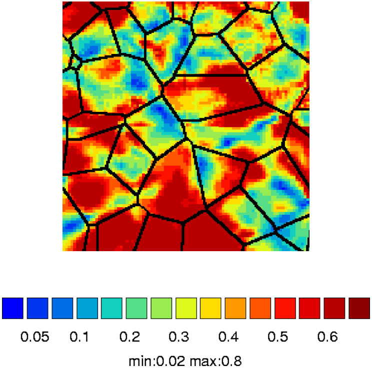
Ensemble average and relative variance

cumulated slip

$\bar{\gamma}_{eq} / < \bar{\gamma}_{eq} >$



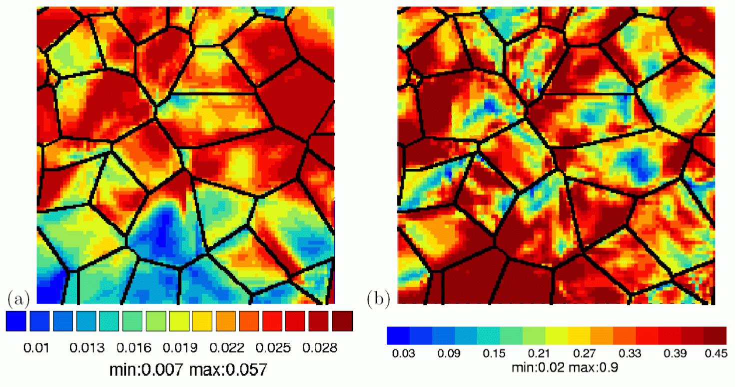
$D(\gamma_{eq})/\bar{\gamma}_{eq}$



Ensemble average and relative variance

lattice rotation field

$\bar{\phi}_c / < \bar{\phi}_c >$ $\quad$ $D(\phi_c)/\bar{\phi}_c$



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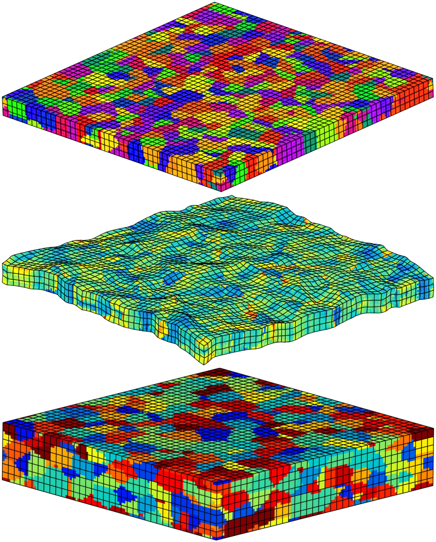
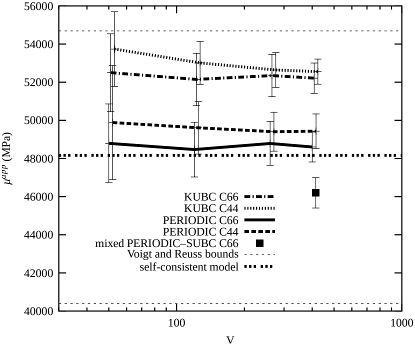
RVE for polycrystalline thin films?



periodic or mixed boundary conditions

The RVE does not exist for a one–grain thick polycrystalline layer

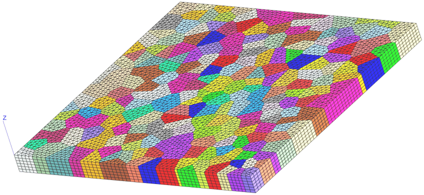


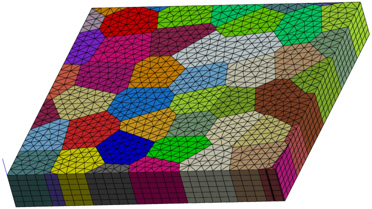
However 3 to 5 grains within the thickness are sufficient to reach bulk properties...
[El Houdaigui, 2004]

Microstructure of the polycrystalline films

columnar grains

relative grain size $d/h = 1$



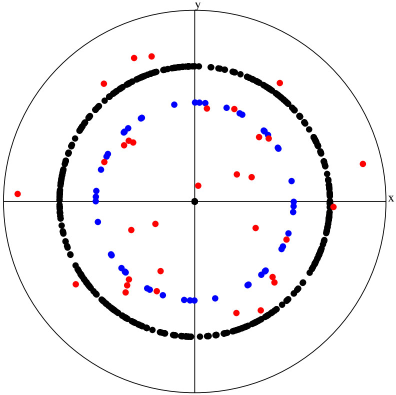


1 realization 225 grains

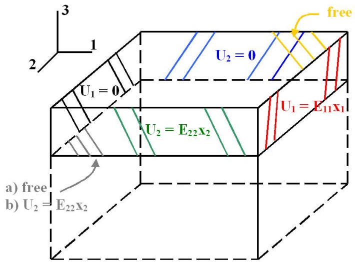
10 realizations 50 grains

[Siska, 2006]

Crystallographic texture and boundary conditions



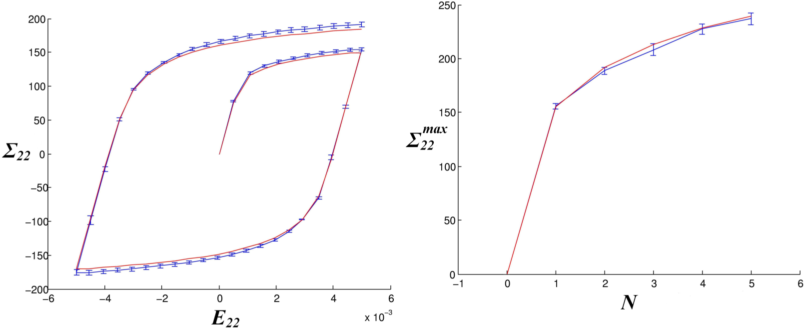
90% {111} grains
6% {001} grains
4% random grains



free–standing film
or
film on a substrate
flat interface

[Siska, 2006]

Overal cyclic response of the films



$$E_{22} = \pm 0.5\%$$

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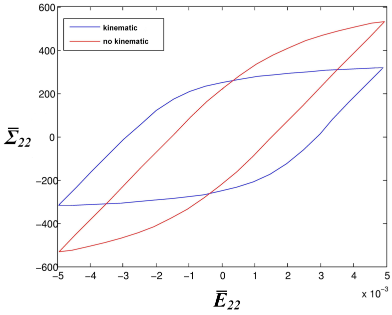
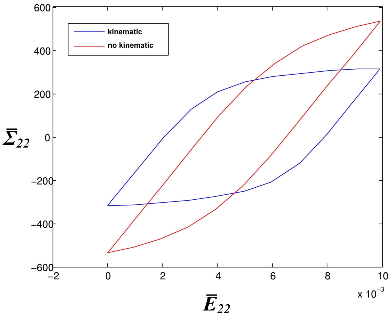
Local vs. overall kinematic hardening

Stabilized overall stress–strain loops for models with and without local kinematic hardening (averaged over 10 realizations of 50–grain aggregates)



cyclic tension–compression

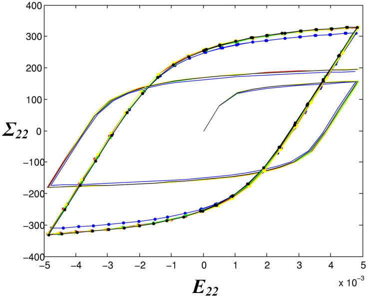
$E_{22} = \pm 0.5\%$

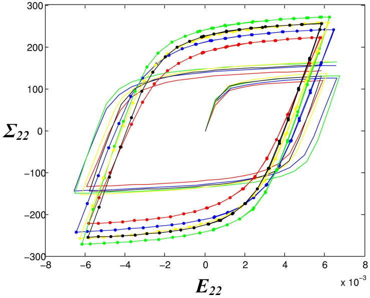


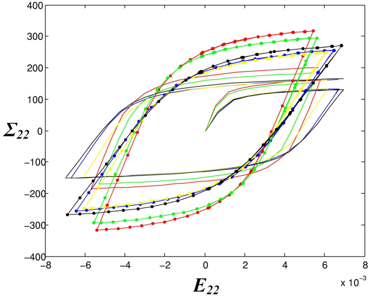
cyclic tension

$E_{22} = 0 - 1\%$

Mean response per texture component

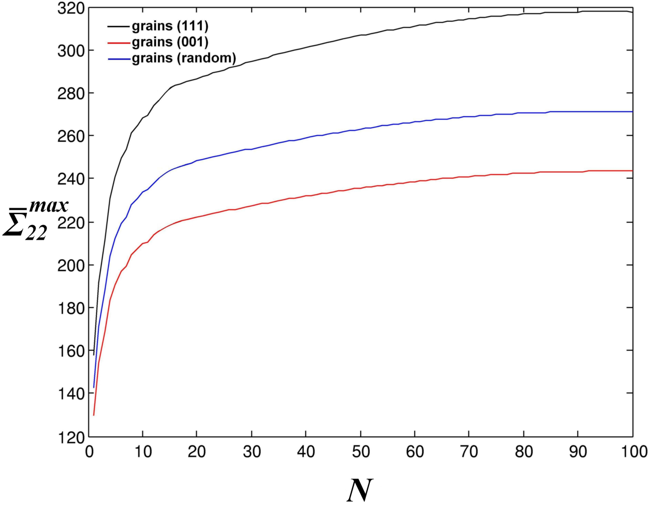






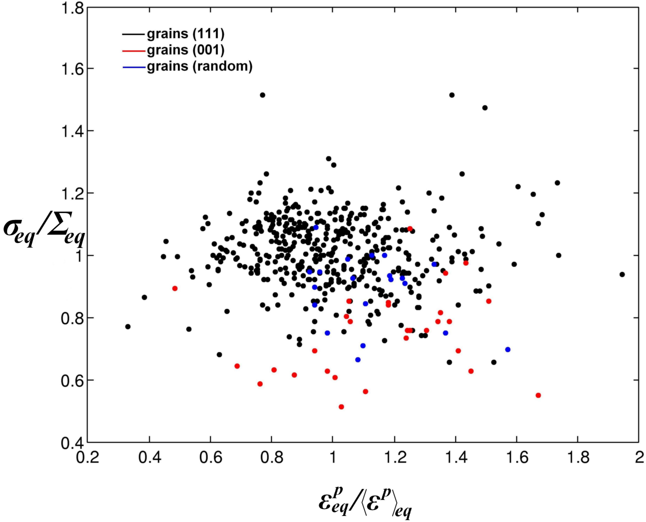
cyclic tension–compression
$E_{22} = \pm 0.5\%$

Cyclic hardening per texture component



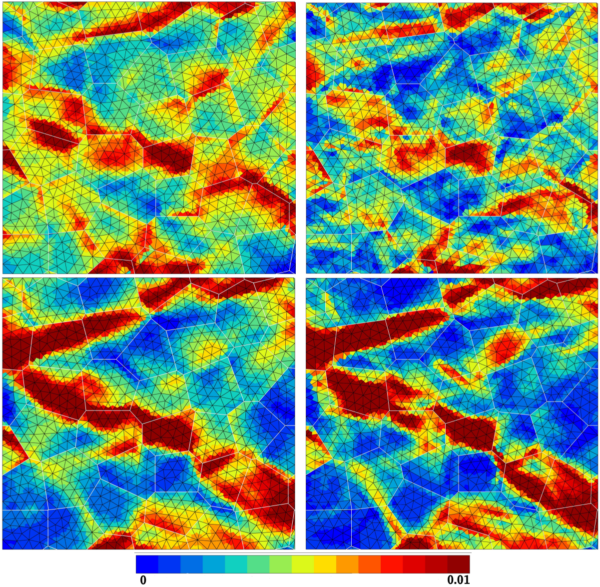
cyclic tension–compression $E_{22} = \pm 0.5\%$

Mean stress/strain per grain after 100 cycles



cyclic tension–compression $E_{22} = \pm 0.5\%$

Plastic strain heterogeneity at the free surface

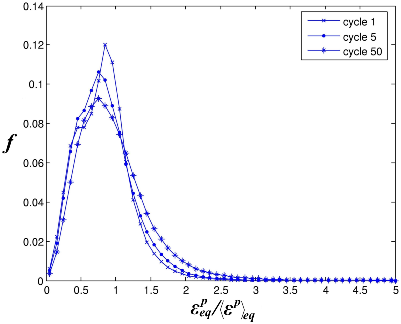


cyclic tension–compression $E_{22} = \pm 0.5\%$

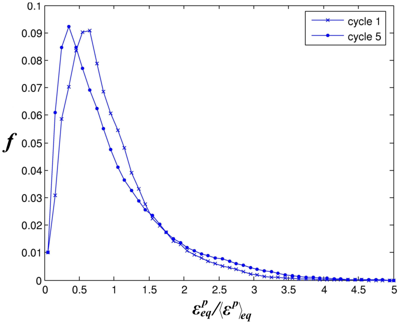
film on a substrate (N=1, 100)

free–standing film (N=1, 100)

Distribution of plastic strain in $\{111\}$ grains



film on a substrate



free–standing film

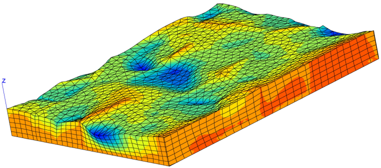
cyclic tension–compression $E_{22} = \pm 0.5\%$

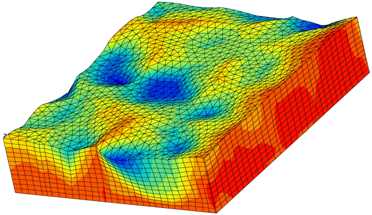
Plan

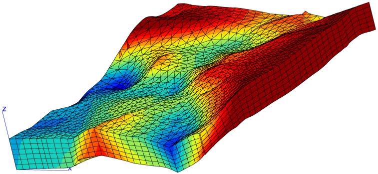
1. Microstructural mechanics
   - Morphology of polycrystalline aggregates
   - Continuum crystal plasticity
   - Validation of the continuum approach
2. Strain heterogeneities in bulk polycrystals
   - Representative volume element size
   - Hierarchy of heterogeneity levels in polycrystals
3. Strain heterogenities at a free surface
   - Range of plastic deformation
   - Impact of 3D grain morphology on surface deformation
   - Ensemble averaging and dispersion of strain field
4. Polycrystalline thin films and coatings
   - Representative volume element for thin films
   - Cyclic behaviour of thin films
   - Plasticity induced roughness
5. Continuum modelling of size effects in polycrystals
   - Enriched grain boundary behaviour
   - Grain size effect

Plasticity induced roughness at the free surface

deformed state after $N = 100$ cycles (magnification $\times 50$)







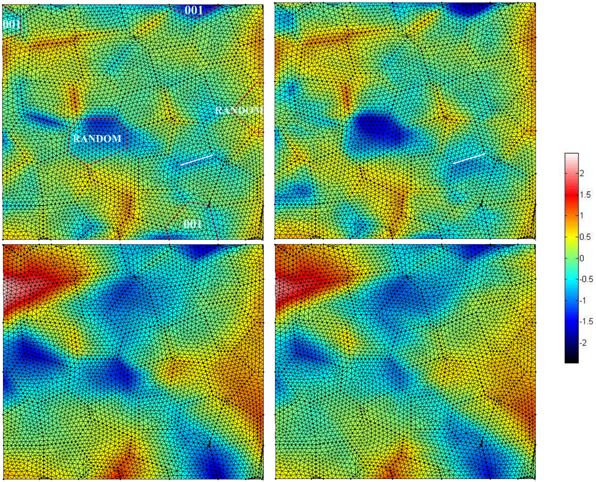
free–standing film

film on a substrate

$d/h = 1$

$d/h = 1/2$

Local roughness maps



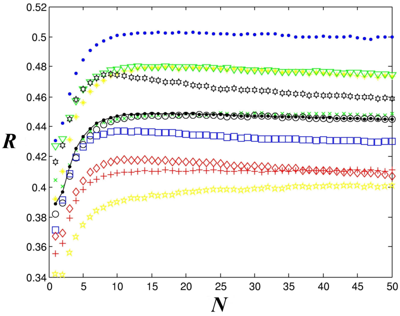
$$R_{loc}(x^i, y^i) =$$

$$\frac{U_3(x^i,y^i) - \overline{U_3}(x^i,y^i)}{|\langle \overline{U_3}(x^i,y^i) \rangle|}$$

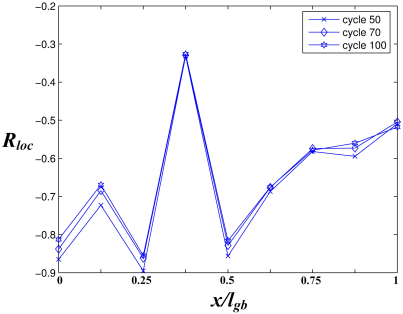
film on a substrate (N=1, 100)

free–standing film (N=1, 100)

Evolution of global and local roughness with cycling



global roughness



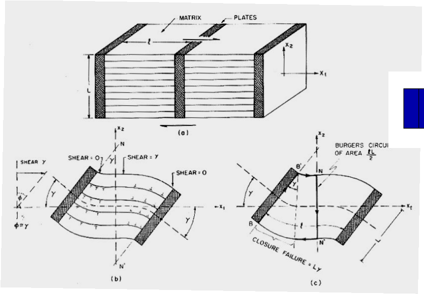
local roughness along a grain boundary

$$R_{RMS} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(U_3(x^i, y^i) - \overline{U_3}(x^i, y^i)\right)^2}, \qquad R = \frac{R_{RMS}}{|\langle \overline{U_3} \rangle|}$$

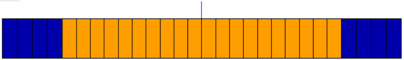
$$R_{loc}(x^i, y^i) = \frac{U_3(x^i, y^i) - \overline{U_3}(x^i, y^i)}{|\langle \overline{U_3}(x^i, y^i) \rangle|}$$

Plan

Plasticity of thin layers



[Ashby, 1970]

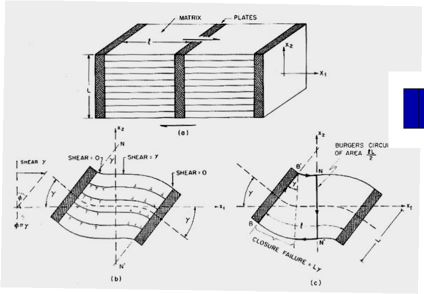


start animate end

periodic simple shear test:
classical solution

classical continuum crystal plasticity cannot account for lattice curvature close to the interface (boundary layer effect)

Plasticity of thin layers



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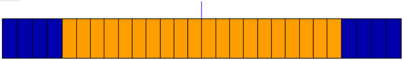

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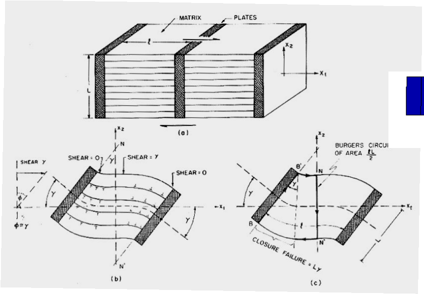

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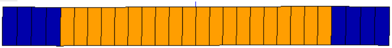

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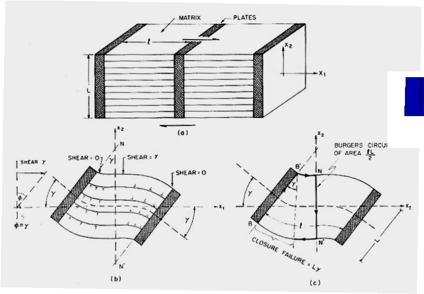

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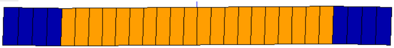

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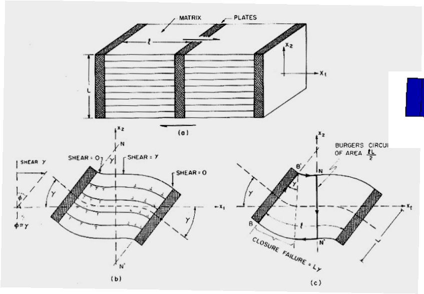

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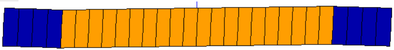

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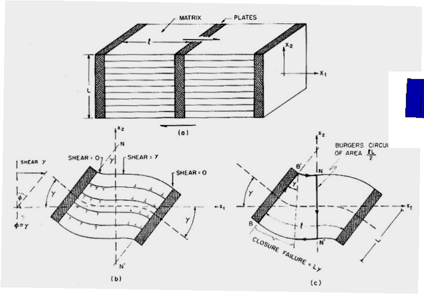

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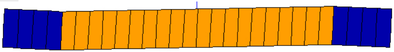

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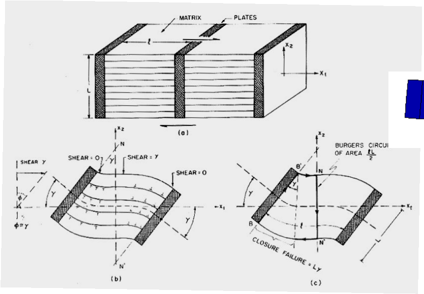

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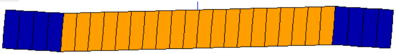

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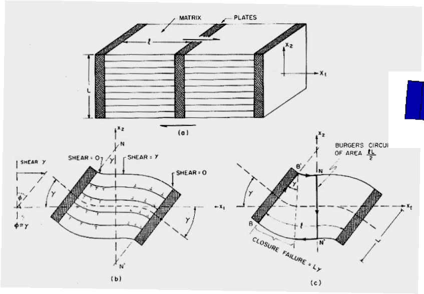

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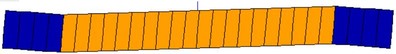

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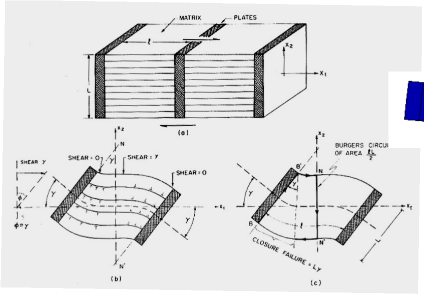

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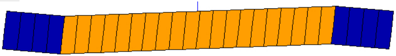

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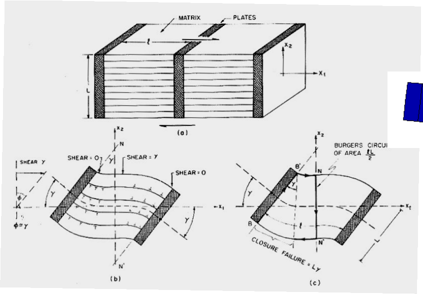

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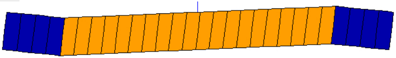

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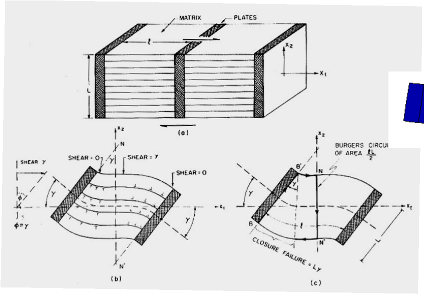

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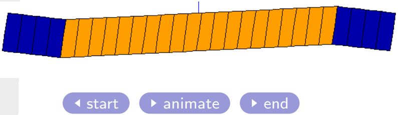

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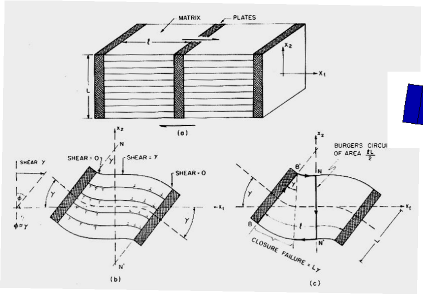

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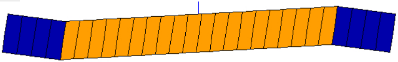

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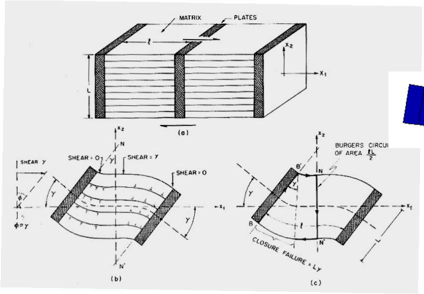

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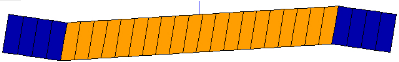

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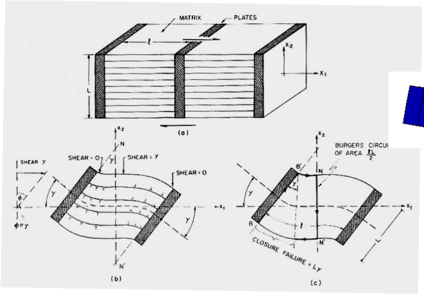

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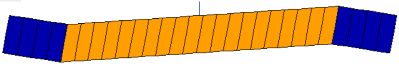

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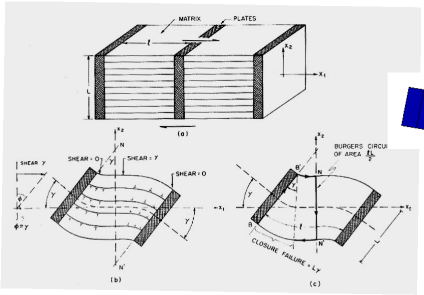

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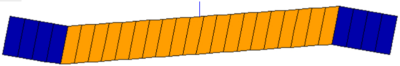

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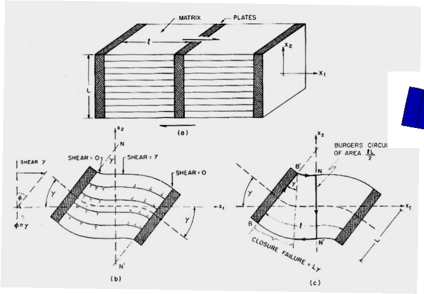

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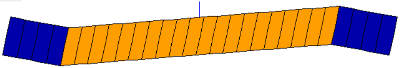

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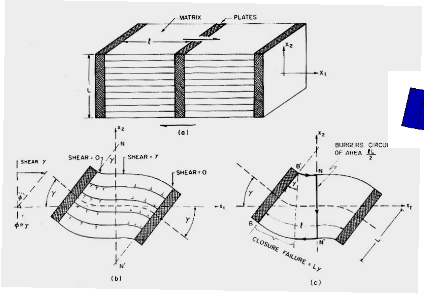

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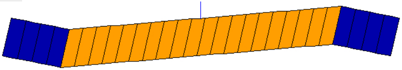

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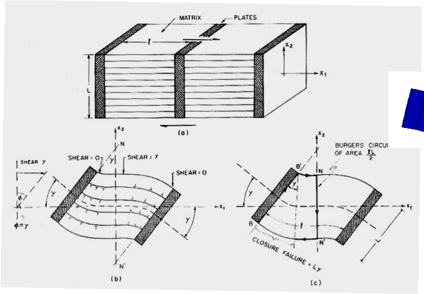

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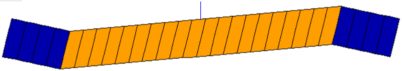

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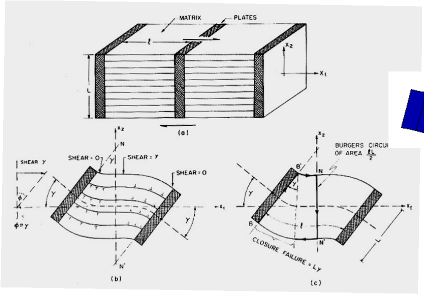

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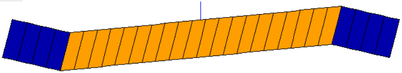

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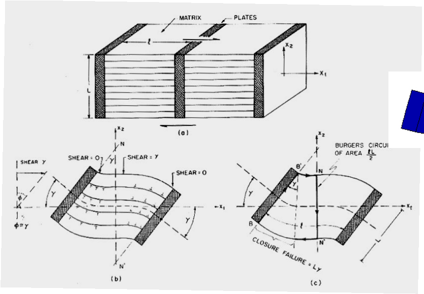

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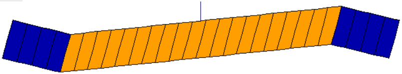

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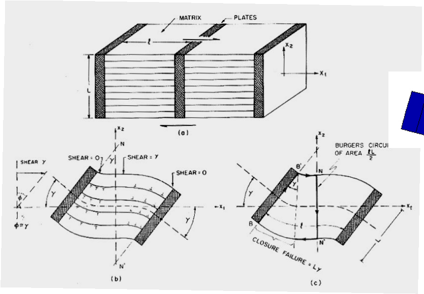

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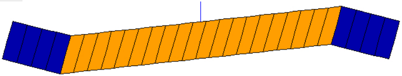

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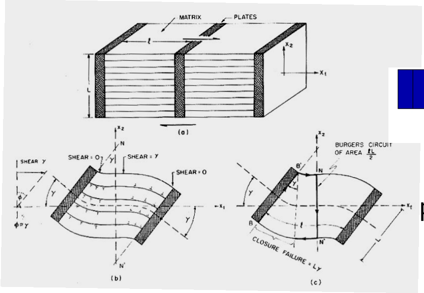

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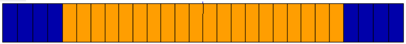
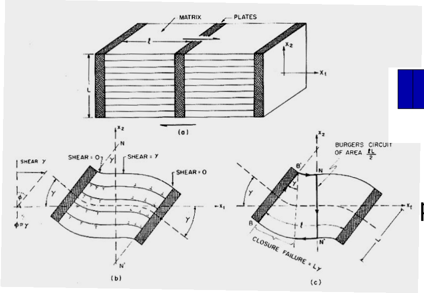


periodic shear test : Cosserat solution (elastic)

Role of continuity requirements at the interface: deisplacement, lattice rotation, stress and couple stress vectors

Plasticity of thin layers



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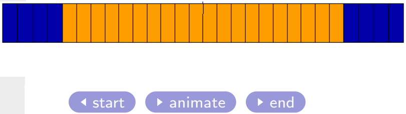

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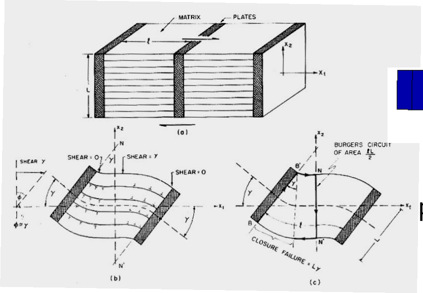
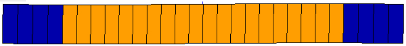
Plasticity of thin layers



[Ashby, 1970]



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periodic shear test : Cosserat solution (elastic)

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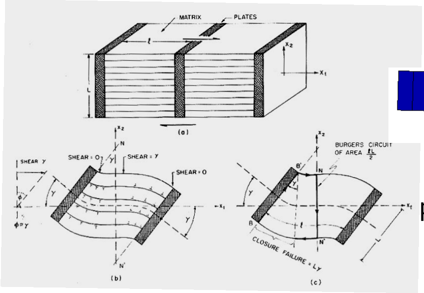

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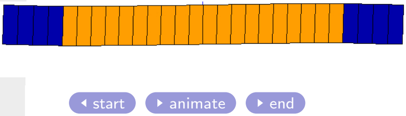

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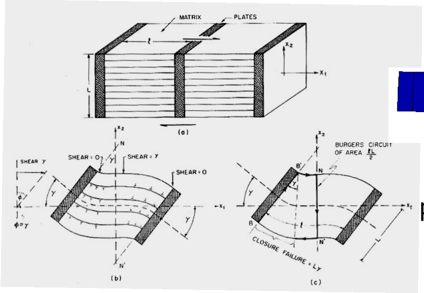

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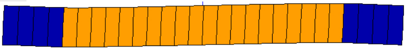

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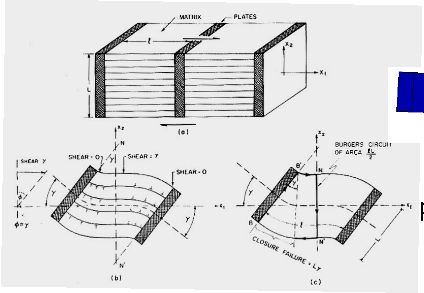

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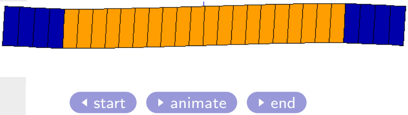

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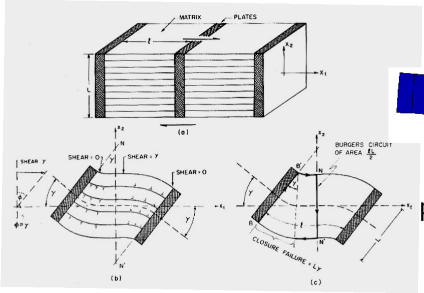

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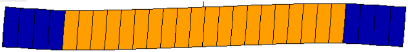

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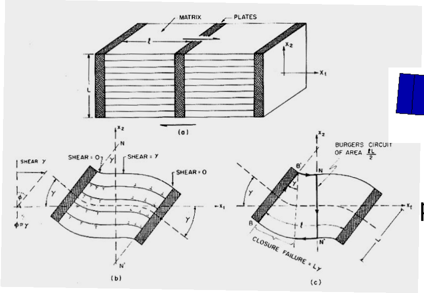

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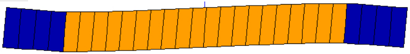

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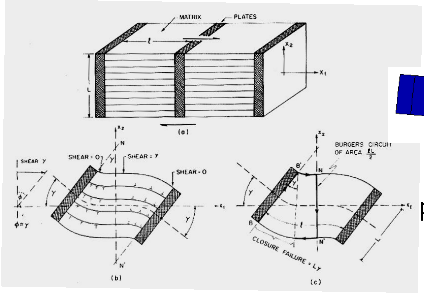

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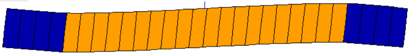

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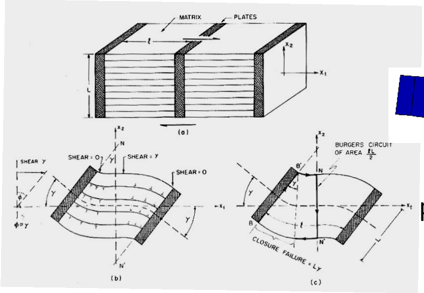

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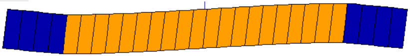

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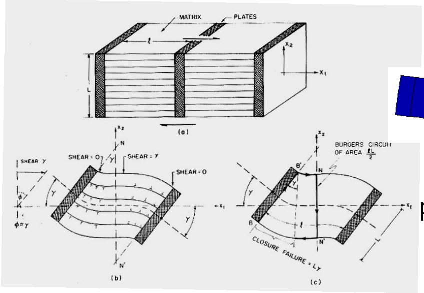

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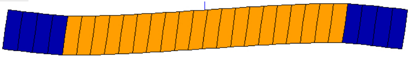

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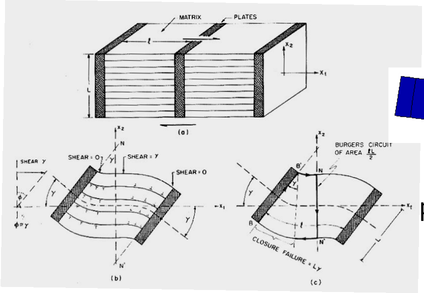

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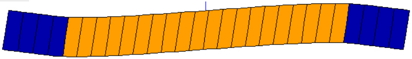

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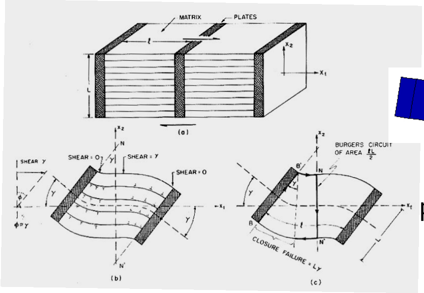

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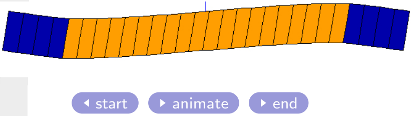

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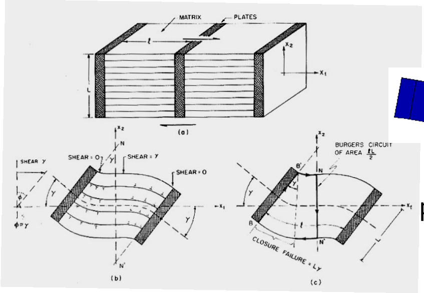

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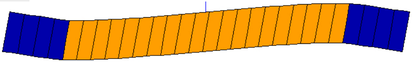

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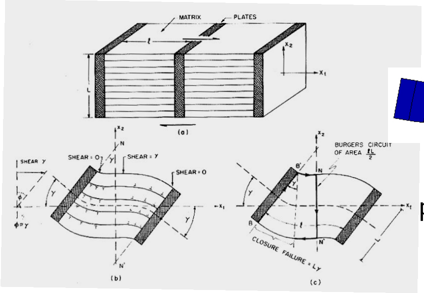

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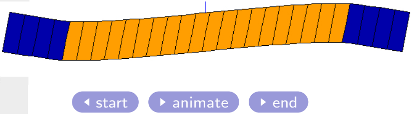

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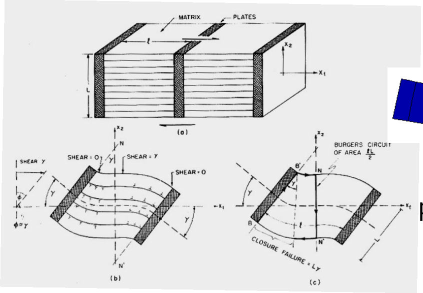

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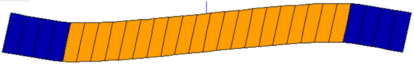

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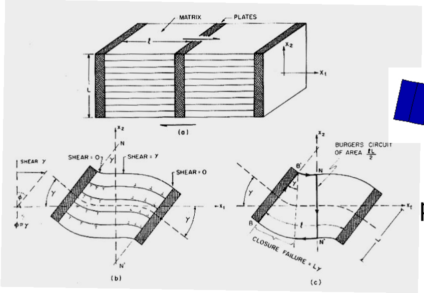

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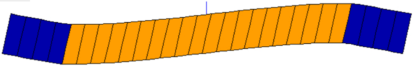

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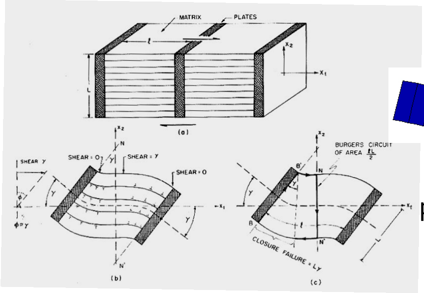

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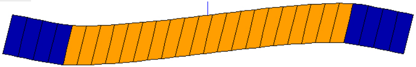

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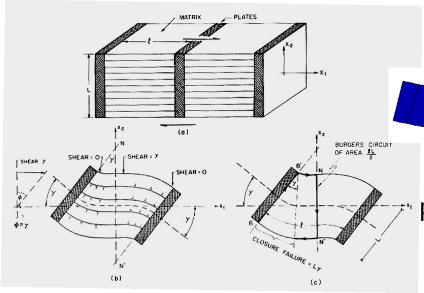

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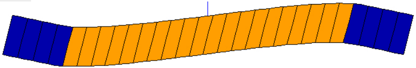

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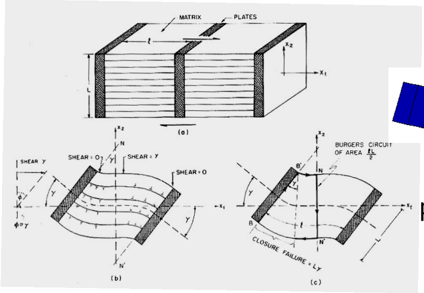

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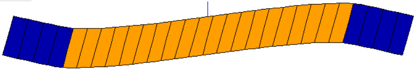

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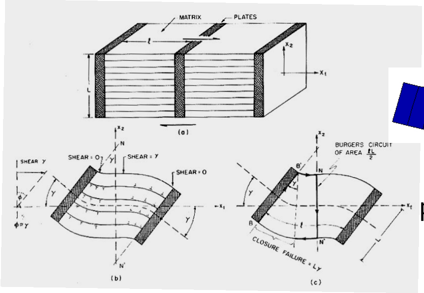

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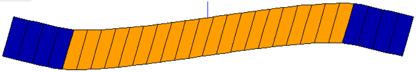

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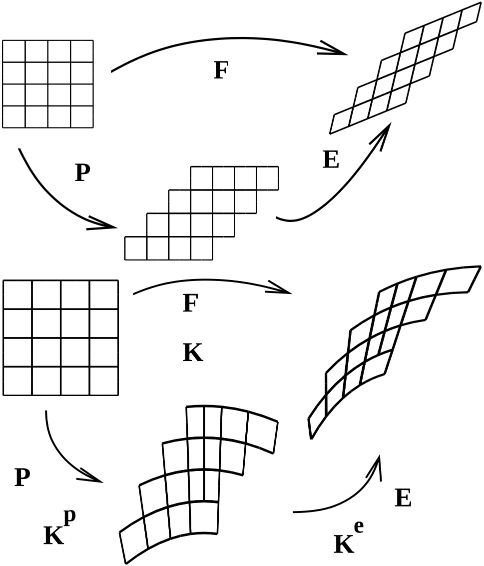
periodic shear test : Cosserat solution (elastic)

Role of continuity requirements at the interface: deisplacement, lattice rotation, stress and couple stress vectors

Dislocation density tensor



resulting Burgers vector

$$\underline{\mathbf{b}} = \oint_c \underset{\sim}{\mathbf{E}}^{-1} . \, d\underline{\mathbf{x}}$$

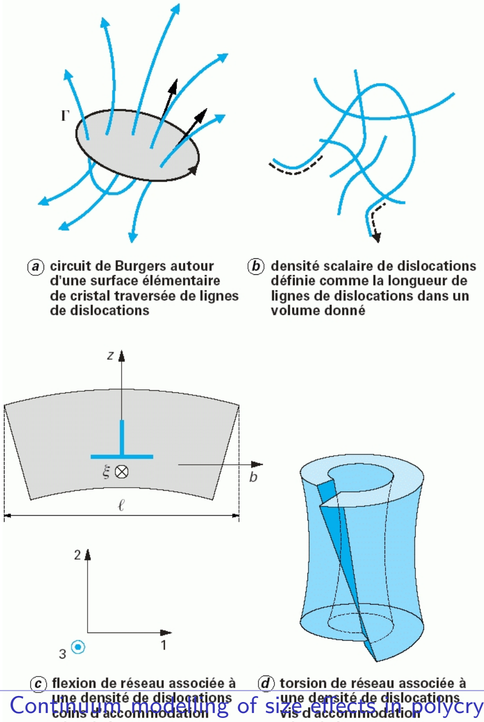
$$\underline{\mathbf{b}} = \int_S \underset{\sim}{\alpha} \, . \underline{\mathbf{n}} \; dS$$

with

$$\underset{\sim}{\alpha} = -\underset{\sim}{\mathbf{curl}} \, \underset{\sim}{\mathbf{E}}^{-1}$$

in other words,

$$\underset{\sim}{\alpha} = < \underline{\mathbf{b}} \otimes \underline{\boldsymbol{\xi}} >$$



Nye's relation (1953)

$$\underset{\sim}{\boldsymbol{\alpha}} = \underset{\sim}{\mathbf{K}}^T - (\operatorname{trace} \underset{\sim}{\mathbf{K}})\underset{\sim}{\mathbf{1}}$$

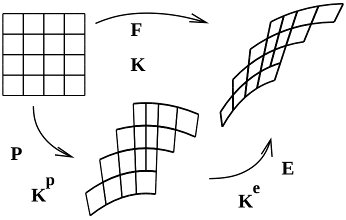
lattice curvature tensor

$$\underset{\sim}{\mathbf{K}} = \underline{\phi} \otimes \boldsymbol{\nabla}$$

lattice curvature due to edge dislocations
lattice torsion due to screw dislocations

Cosserat crystal plasticity model

$$ {}^\sharp\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{R}}^T . \underset{\sim}{\mathbf{F}}, \quad {}^\sharp\underset{\sim}{\mathbf{K}} = \underset{\sim}{\mathbf{R}}^T . \underset{\sim}{\mathbf{K}} $$



multiplicative/additive decomposition

$$ {}^\sharp\underset{\sim}{\mathbf{F}} = {}^\sharp\underset{\sim}{\mathbf{F}}^e . {}^\sharp\underset{\sim}{\mathbf{F}}^p, \qquad {}^\sharp\underset{\sim}{\mathbf{K}} = {}^\sharp\underset{\sim}{\mathbf{K}}^e . {}^\sharp\underset{\sim}{\mathbf{F}}^p + {}^\sharp\underset{\sim}{\mathbf{K}}^p $$

$$ {}^\sharp\dot{\underset{\sim}{\mathbf{F}}}^p . {}^\sharp\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s=1}^{n} \dot{\gamma}^s \, {}^\sharp\underset{\sim}{\mathbf{P}}^s $$

$$ {}^\sharp\dot{\underset{\sim}{\mathbf{K}}}^p . {}^\sharp\underset{\sim}{\mathbf{F}}^{p-1} = \sum_{s=1}^{n} \left(\frac{\dot{\theta}^s_\perp}{l_\perp} {}^\sharp\underset{\sim}{\mathbf{Q}}^s{}_\perp + \frac{\dot{\theta}^s_\odot}{l_\odot} {}^\sharp\underset{\sim}{\mathbf{Q}}^s{}_\odot \right) $$

$$ {}^\sharp\underset{\sim}{\mathbf{P}}^s = {}^\sharp\underline{\mathbf{m}}^s \otimes {}^\sharp\underline{\mathbf{n}}^s $$

$$ {}^\sharp\underset{\sim}{\mathbf{Q}}_\perp = {}^\sharp\underline{\boldsymbol{\xi}} \otimes {}^\sharp\underline{\mathbf{m}}, \; {}^\sharp\underset{\sim}{\mathbf{Q}}_\odot = \frac{1}{2}\underset{\sim}{\mathbf{1}} - {}^\sharp\underline{\mathbf{m}} \otimes {}^\sharp\underline{\mathbf{m}} $$

generalized Schmid law

$$ \tau^s = \underset{\sim}{\mathbf{P}}^s : \underset{\sim}{\boldsymbol{\sigma}}^s $$

$$ \nu^s = \underset{\sim}{\mathbf{Q}}^s : \underset{\sim}{\boldsymbol{\mu}}^s $$

$$ \dot{\gamma}^s = < \frac{|\,\tau^s\,| - r^s}{k} >^n \operatorname{sign}\tau^s $$

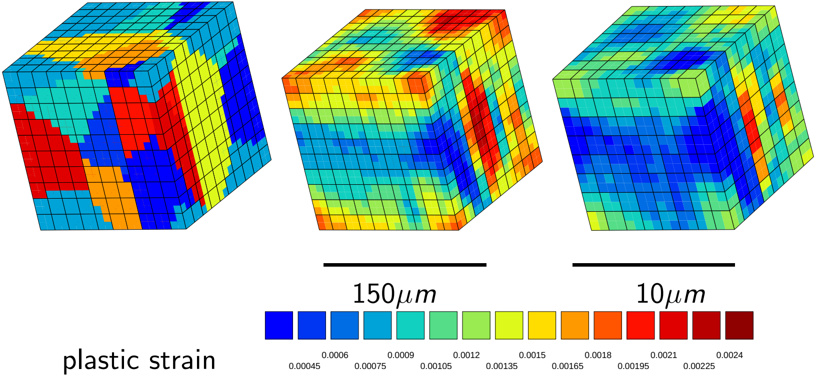
$$ \dot{\theta}^s = < \frac{|\,\nu^s\,| - l_\perp r_c^s}{l_\perp k_c} >^{n_c} \operatorname{sign}(\nu^s) $$

hardening law

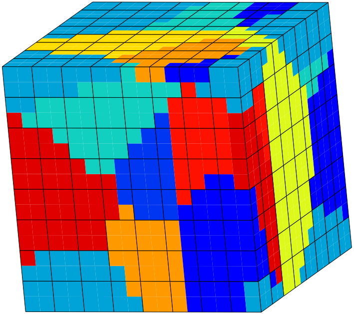
$$ r^s = r_0 + q \sum_{r=1}^{n} h^{sr}(1 - \exp(-bv^r)) + R(|\,\theta^s\,|), \qquad r_c^s = r_{c0} $$

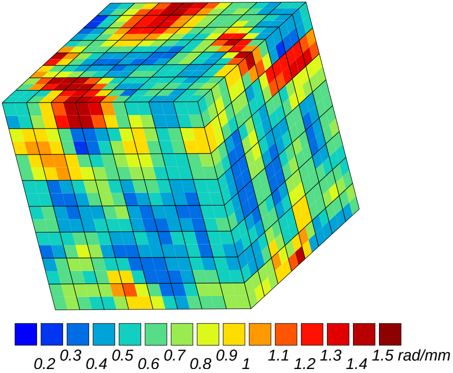
Plan

Grain size effects in polycrystals



Lattice curvature in a ferritic steel





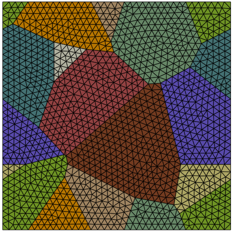
$\simeq 1 - 10^\circ/\mu m$

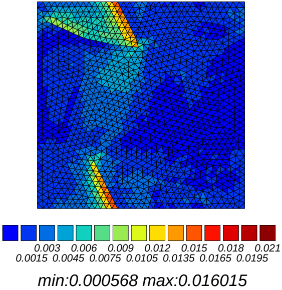
additional hardening $R^s(\theta^s) = Q_c \sqrt{\sum_r |\theta^r|}$

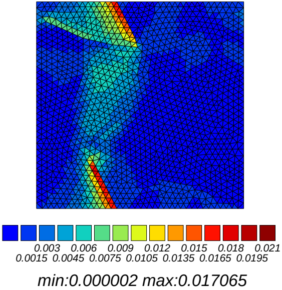
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: plastic strain





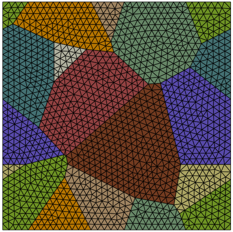


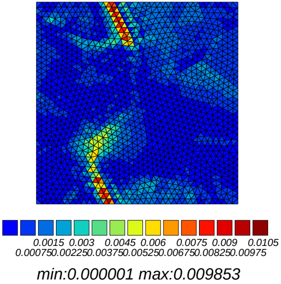
$150\mu m$ $10\mu m$

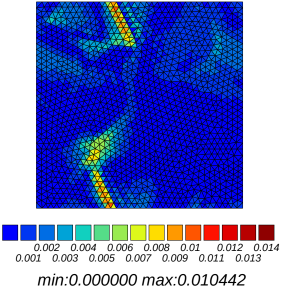
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: lattice rotation





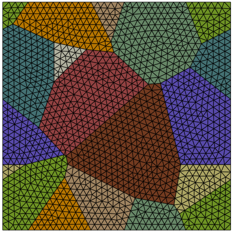


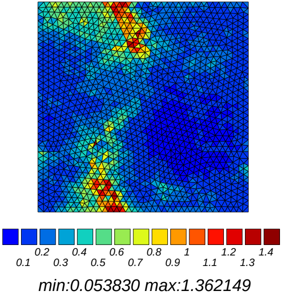
$150\mu m$ $\qquad$ $10\mu m$

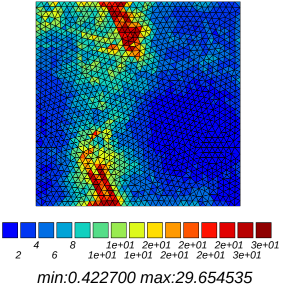
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: lattice curvature





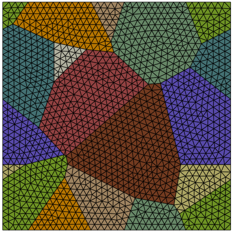


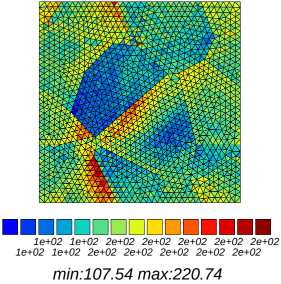
$150\mu m$ $\qquad$ $10\mu m$

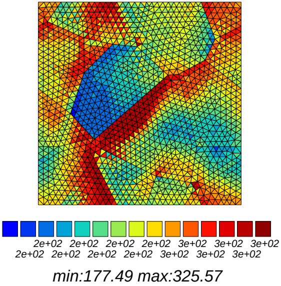
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity : local stresses





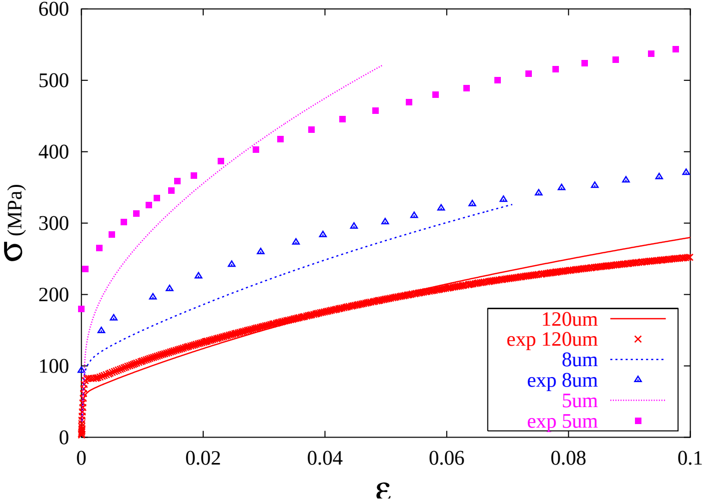


$150\mu m$ $10\mu m$

additional hardening $R^s(\theta^s) = Q_c \sqrt{\sum_r |\theta^r|}$

[Zeghadi, 2004]

Grain size effects in a ferritic steel



[Bouaziz, 2002]

Open problems

- Experimental needs:
  - ⋆ systematic 3D "EBSD" measurements
  - ⋆ systematic 3D elastic strain tensor components measurements
  - ⋆ measuring 3D total strain components?
- Computational improvements:
  - ⋆ larger volume element size and finer meshes
  - ⋆ statistical orientation distribution models taking grain neighbour misorientations into account
  - ⋆ realistic size–dependent constitutive models, possibly based on generalized continuum models (strain gradient plasticity or Cosserat...)
  - ⋆ links with DDD simulations to account for slip line or PSB formation
  - ⋆ links with DDD and atomistics and TEM for a better description of dislocation grain boundary interaction
  - ⋆ incorporate other mechanisms like *twinning*