Modeling relative and absolute size effects in crystal plasticity

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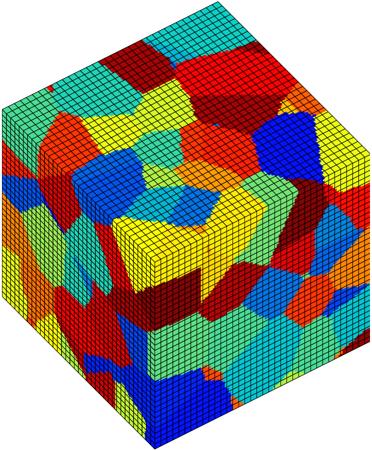
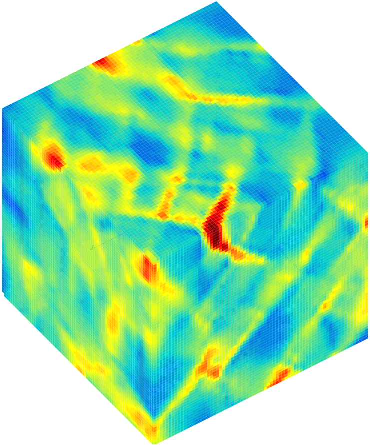
Plan

1. Representative volume element sizes for polycrystals
   - Bulk copper
   - Copper thin sheets
   - Equiaxial vs. pancake grains in zinc coatings
2. Grain size effect in polycrystals
   - Cosserat single crystal plasticity
   - Homogenization of Cosserat media
   - Hall–Petch effect in ferritic steels
3. Conclusions

Computations of polycrystalline aggregates



RVE of the polycrystal



equivalent plastic strain

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Boundary conditions

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

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

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

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

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

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

- **Periodicity conditions (PERIODIC)** :

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

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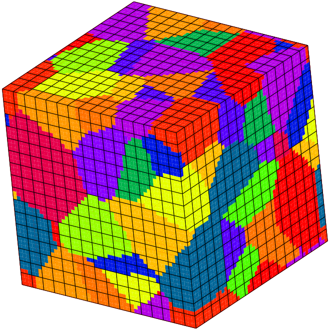
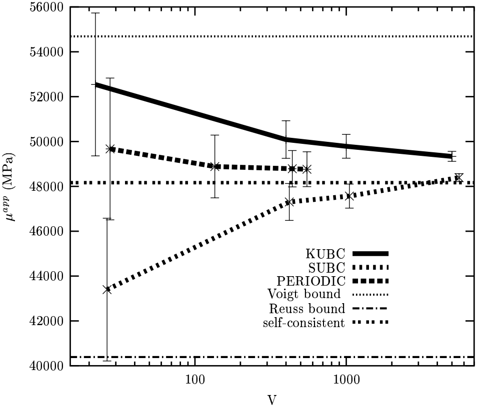
RVE size for elastic isotropic bulk copper polycrystals





$C_{11} = 168400$ MPa, $\quad C_{12} = 121400$ MPa, $\quad C_{44} = 75390$ MPa, $a = 2C_4$

RVE size and integral range

$Z(x)$ a local random variable (volume fraction, Young's modulus, ...)
The variance $D_Z^2(V)$ of apparent property Z for a volume V is taken as

$$D_Z^2(V) = D_Z^2 \frac{A_3}{V}$$

where D_Z^2 the local variance of Z :

$$D_Z^2 = P(1-P) \text{ for volume fraction } (Z = P)$$
$$D_\mu^2 = P(1-P)(\mu_1 - \mu_2)^2 \text{ for a two–phase material}$$

and A_3 is the integral range

For volume fraction ($Z = P$) and Voronoi mosaics, $\alpha = 1$ and
$A_3 = 1.18$ [Gilbert, 1962]
for elastic bulk copper polycrystals $A_3 = 1.43$

Statistical definition of the RVE

For a sufficiently large number n of realizations, the mean apparent property $\bar{Z}$ lies in the interval of confidence

$$Z^{eff} \pm \frac{2D_Z(V)}{\sqrt{n}}$$

The relative precision on the mean is therefore :

$$\epsilon_{rel} = \frac{2D_Z(V)}{\sqrt{n}Z^{eff}} = \frac{2D_Z\sqrt{(\frac{A_3}{V})^{\alpha}}}{\sqrt{n}Z^{eff}}$$

For given precision and number of realizations, the size of the RVE is defined as

$$V_{\mathrm{RVE}} = A_3 \left(\frac{4D_Z^2}{n\epsilon_{rel}^2 Z^{eff}} \right)$$

[Kanit *et al.*, 2003]

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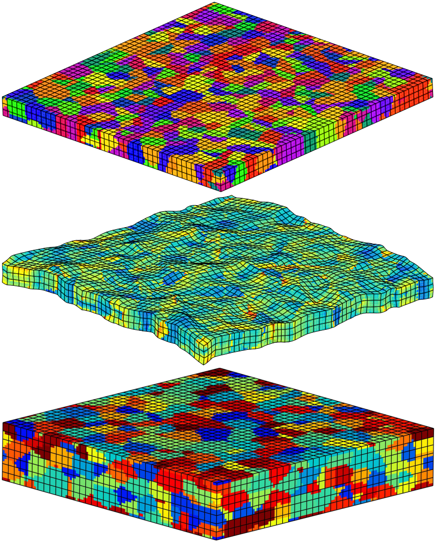
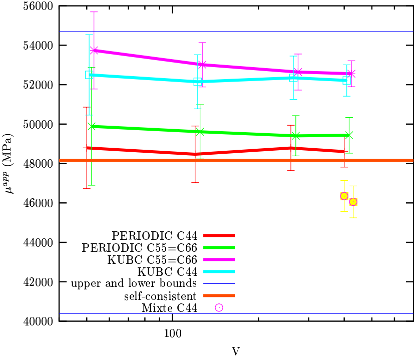
RVE size and thin sheets



periodic or mixt boundary conditions

the RVE does not exist for one–grain thick sheets



but 3 to 5 grains through the thickness are sufficient to reach bulk properties…

[El Houdaigui, 2004]

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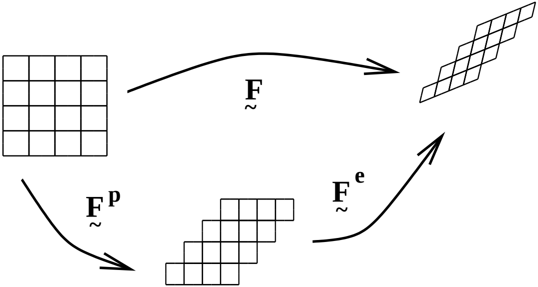
Continuum crystal plasticity theory

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

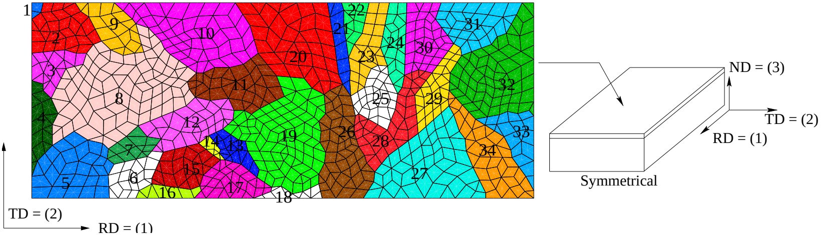
$$\tau^s = \underset{\sim}{\mathbf{P}}^s : \underset{\sim}{\boldsymbol{\sigma}}^s$$

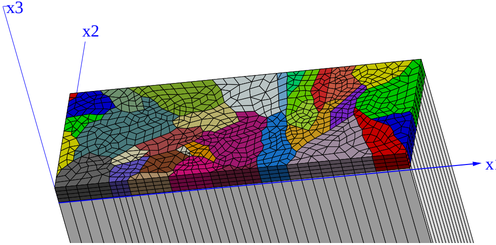
$$\dot{\gamma}^s = < \frac{\mid \tau^s \mid - r^s}{k} >^n \mathrm{sign}\tau^s$$

Hardening law

$$r^s = r_0 + q \sum_{r=1}^{n} h^{sr} (1 - \exp(-bv^r))$$

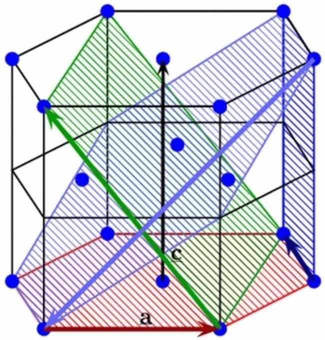
Mechanical behaviour of zinc coatings in galvanized steel sheets





- in–plane grain size d,
- coating thickness $h = 10\ \mu$m,
- investigate ratio $d/h = 1$ (equiaxial) and 50 (pancakes)

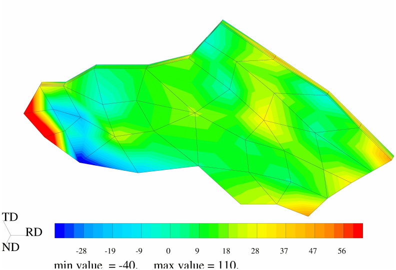
Deformation mechanisms in zinc coatings



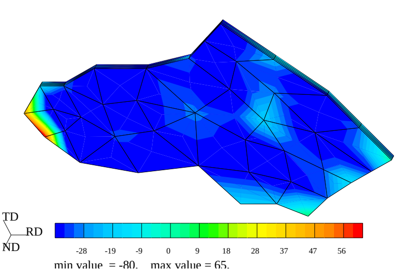
- H.C.P avec c/a=1.856
- Glissement Basal $(0001) < 11\bar{2}0 >$
- Glissement Prismatique $\{1\bar{1}00\} < 11\bar{2}0 >$
- Glissement Pyramidal π_2 $\{\bar{1}\bar{1}23\} < 11\bar{2}3 >$
- Maclage $\{10\bar{1}2\} < 10\bar{1}\bar{1} >$
  Maclage par compression selon l'axe **c**

Substrate effect on pancake grains

σ_{11} in grain 11



σ_{22} in grain 11



tensile test in grain 11:

$$\begin{bmatrix} \varepsilon^p & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\varepsilon^p \end{bmatrix}$$

steel sheet in tension:

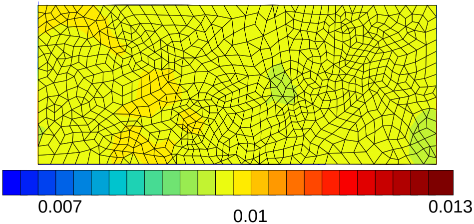
$$\begin{bmatrix} \varepsilon^p & 0 & 0 \\ 0 & -\varepsilon^p/2 & 0 \\ 0 & 0 & -\varepsilon^p/2 \end{bmatrix}$$

$\Longrightarrow$ biaxial stress state in grain 11 on the substrate:

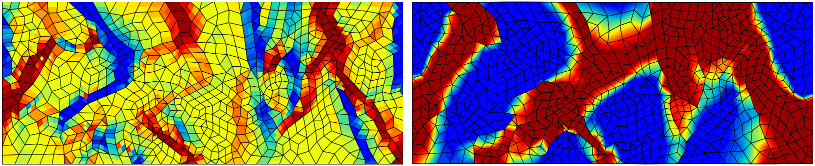
$$\begin{bmatrix} \sigma & 0 & 0 \\ 0 & \simeq -3\sigma & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Relative grain size effect in zinc coatings

ε_{11} at the interface

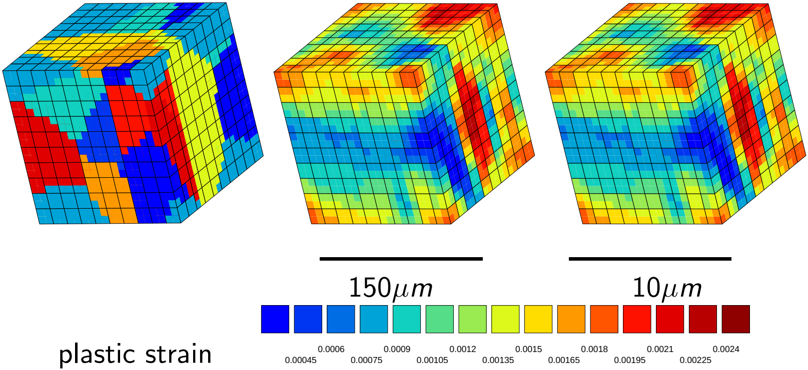


pancake grains ε_{11} at the free surface equiaxial grains



Plan

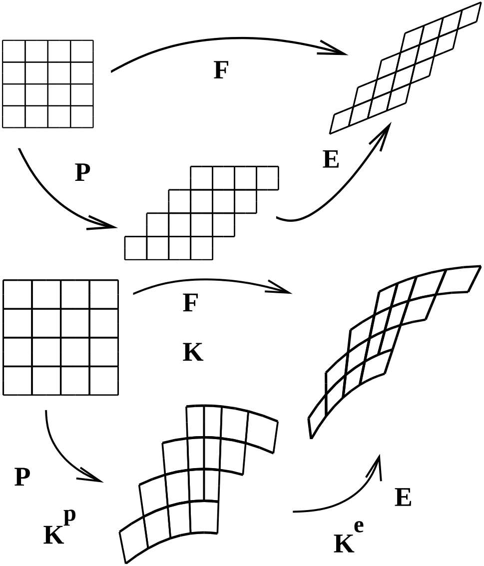
Grain size effect in polycrystals



In classical continuum crystal plasticity there is no absolute grain size effect $\neq$ physical metallurgy!

Plan

Dislocation density tensor



resulting Burgers vector

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

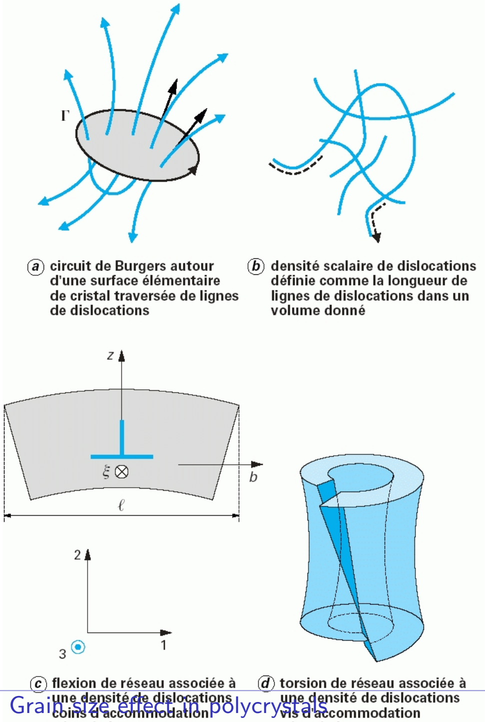
$$\underline{\mathbf{b}} = \int_{S} \underset{\sim}{\boldsymbol{\alpha}} \, . \underline{\mathbf{n}} \, dS$$

with

$$\underset{\sim}{\boldsymbol{\alpha}} = -\mathbf{c}\underset{\sim}{\mathbf{u}}\mathbf{rl} \, \underset{\sim}{\mathbf{E}}^{-1}$$

in other words,

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



Nye's relation (1953)

$$\underset{\sim}{\alpha} = \underset{\sim}{K}^T - (\mathrm{trace}\,\underset{\sim}{K})\underset{\sim}{1}$$

lattice curvature tensor

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

lattice curvature due to edge dislocations
lattice torsion due to screww dislocations

Cosserat crystal plasticity model

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

multiplicative/additive decomposition

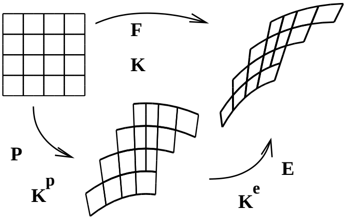
$$^\sharp\underset{\sim}{F} = {}^\sharp\underset{\sim}{F}^e . {}^\sharp\underset{\sim}{F}^p, \qquad ^\sharp\underset{\sim}{K} = {}^\sharp\underset{\sim}{K}^e . {}^\sharp\underset{\sim}{F}^p + {}^\sharp\underset{\sim}{K}^p$$

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

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

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

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



generalized Schmid law

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

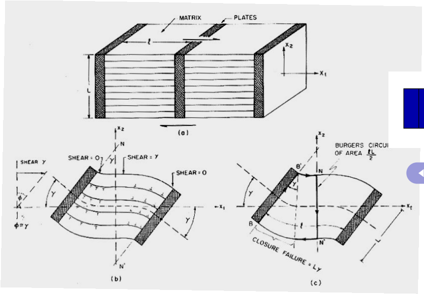
$$\nu^s = \underset{\sim}{Q}^s : \underset{\sim}{\mu}^s$$

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

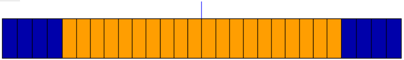
$$\dot{\theta}^s = < \frac{|\nu^s| - l_\perp r^s_c}{l_\perp k_c} >^{n_c} \operatorname{sign}(\nu^s)$$

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

Plasticity of thin layers



[Ashby, 1970]



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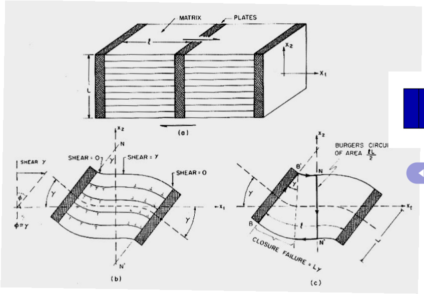
periodic simple shear test: classical solution

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

Plasticity of thin layers



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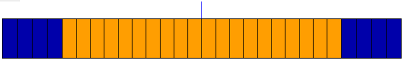

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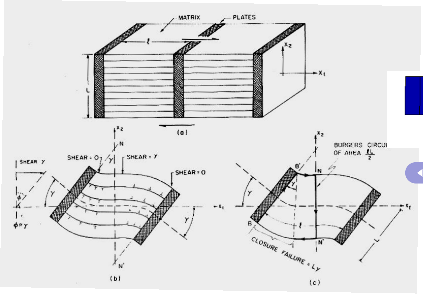

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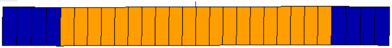

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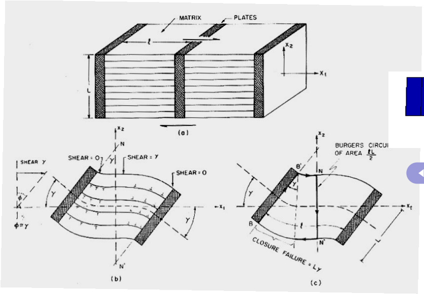

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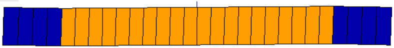

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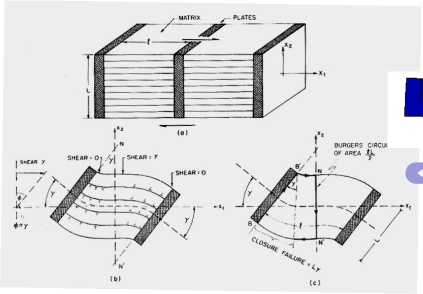

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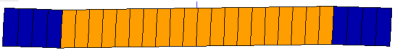

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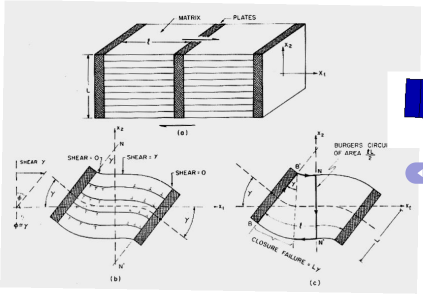

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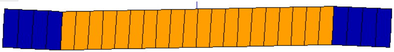

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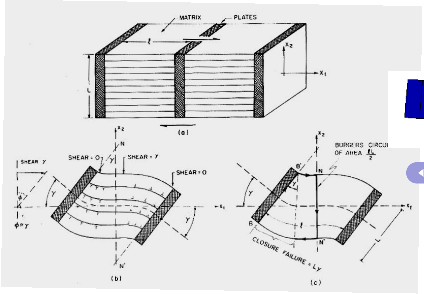

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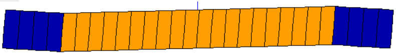

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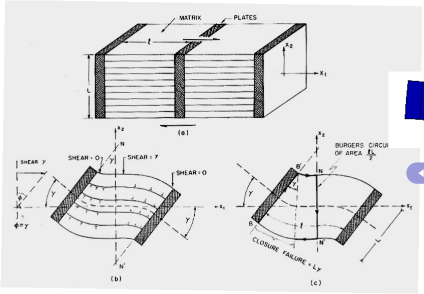

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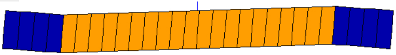

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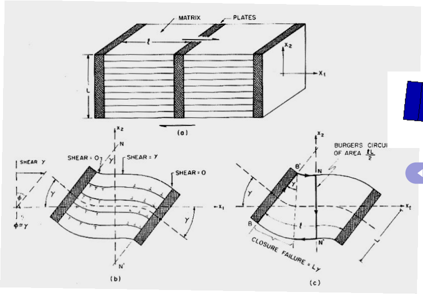

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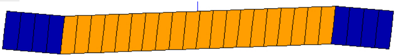

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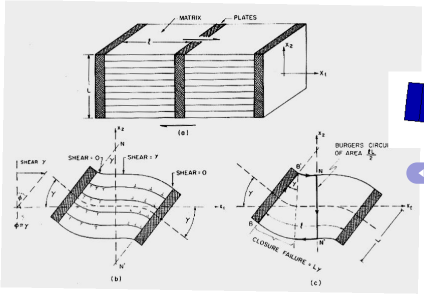

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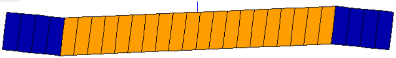

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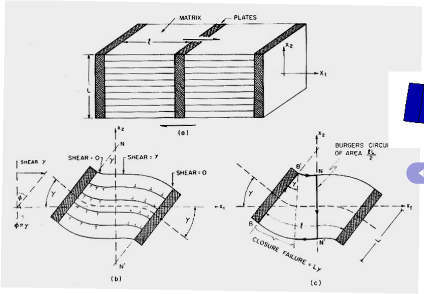

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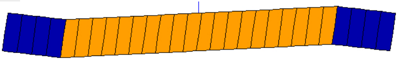

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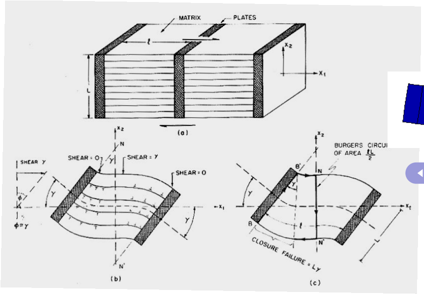

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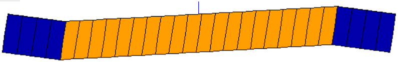

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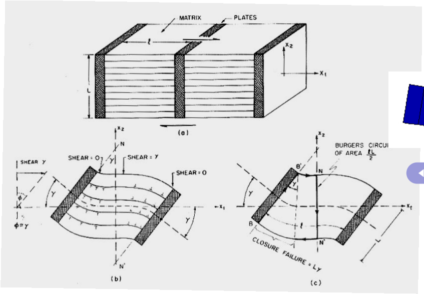
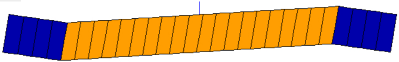


[Ashby, 1970]



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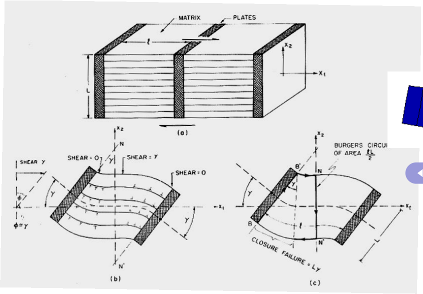
periodic simple shear test: classical solution

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

Plasticity of thin layers



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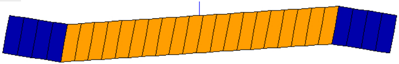

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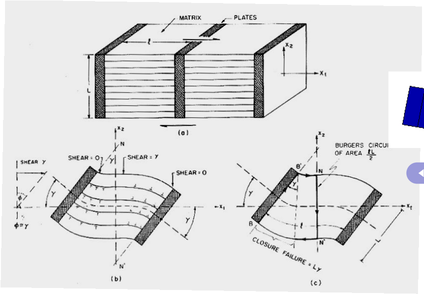

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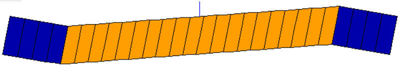

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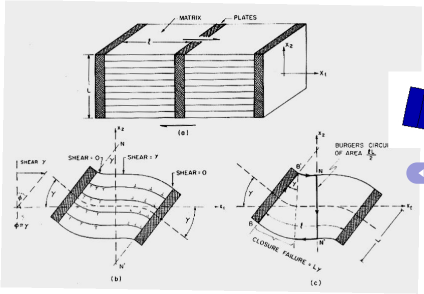

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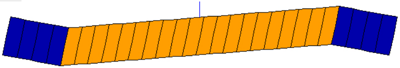

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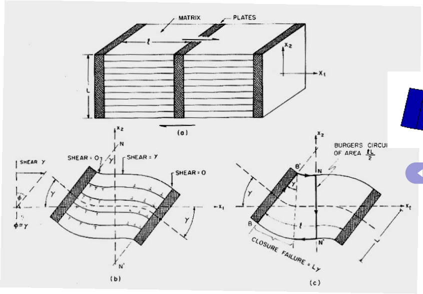

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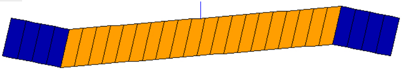

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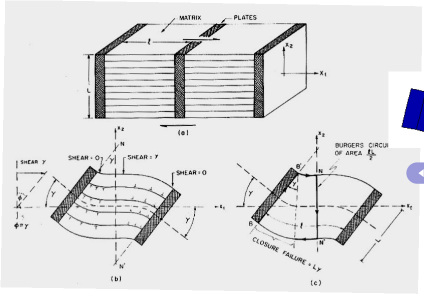

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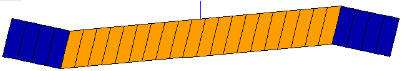

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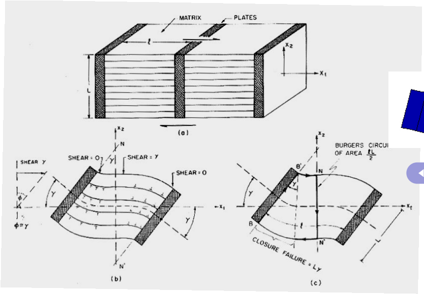

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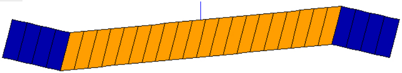

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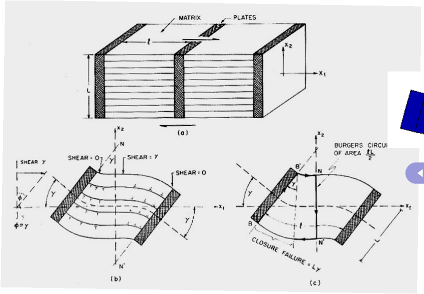

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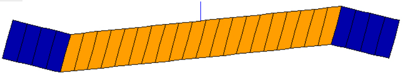

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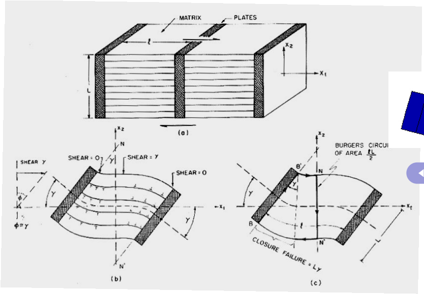

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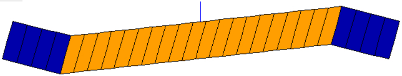

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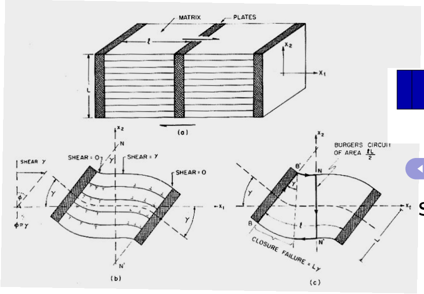

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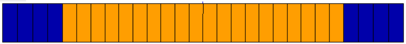

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periodic shear test : Cosserat solution (elastic)

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

[Forest, Sedlacek 2003]

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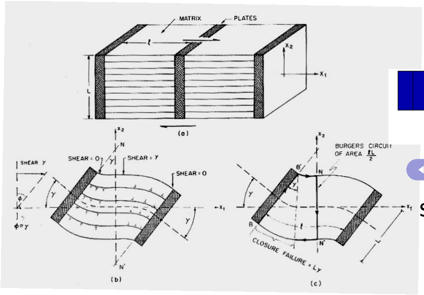

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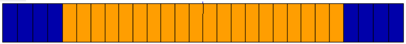

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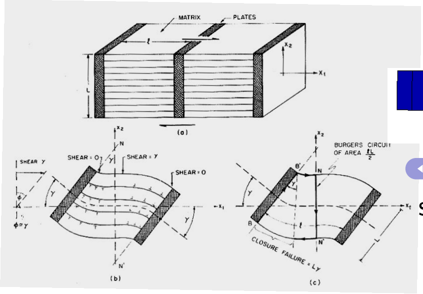

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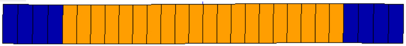

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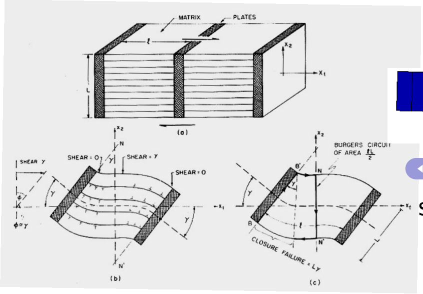

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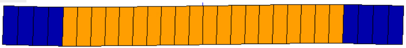

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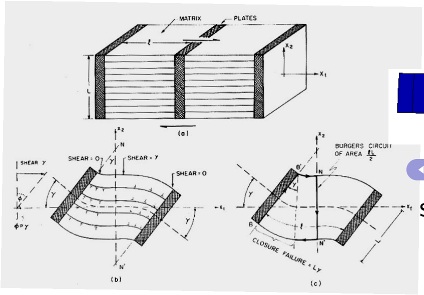

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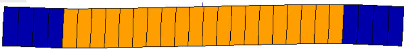

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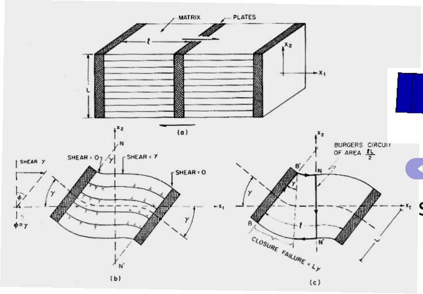

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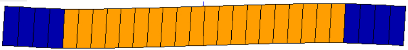

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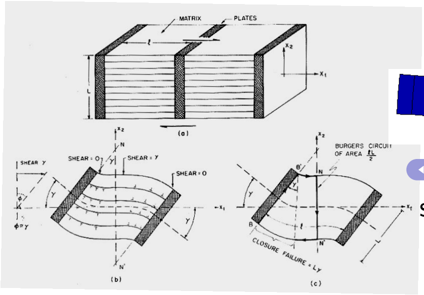

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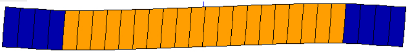

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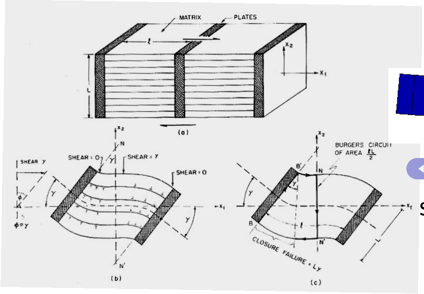

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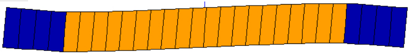

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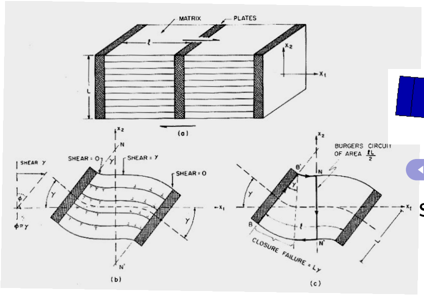

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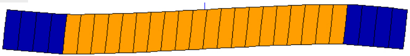

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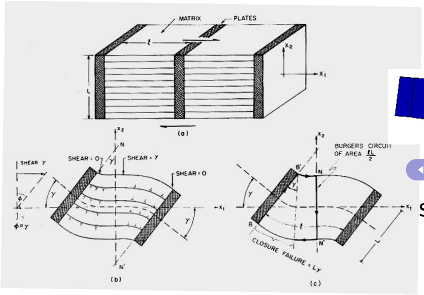

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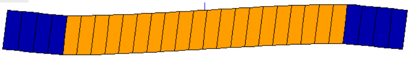

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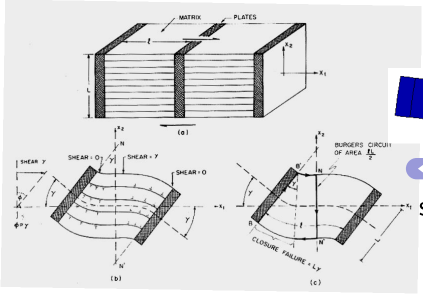

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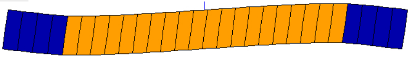

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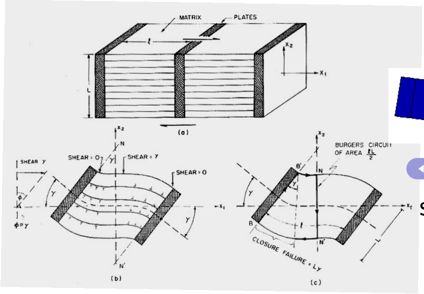

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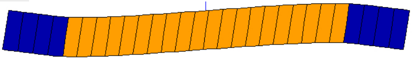

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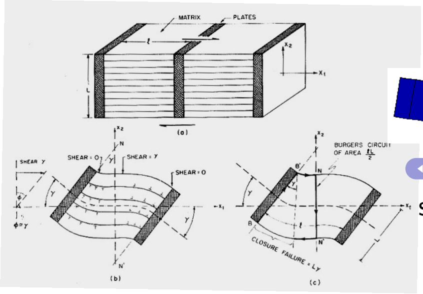

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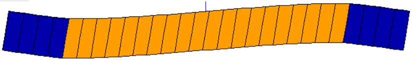

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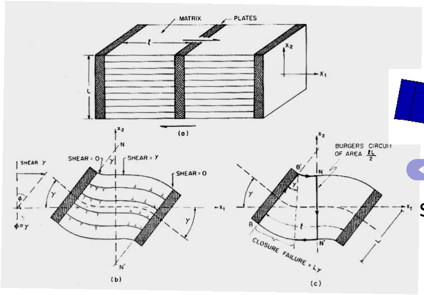

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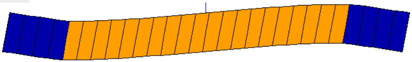

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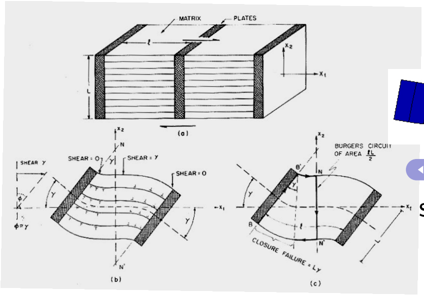

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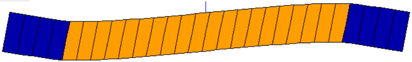

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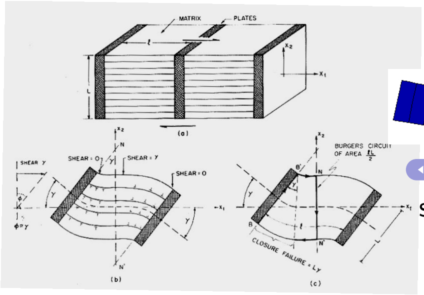

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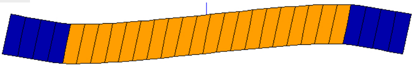

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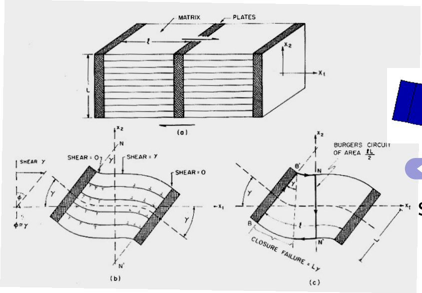

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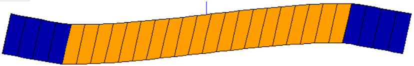

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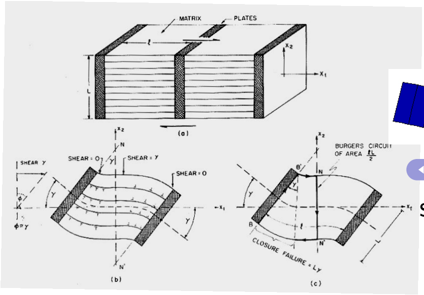

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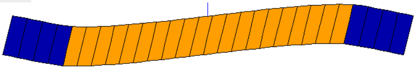

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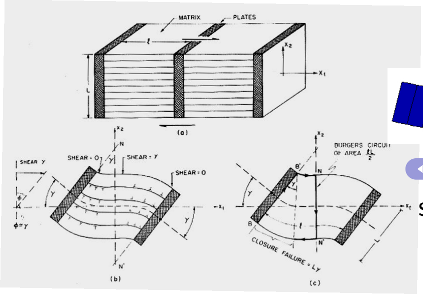

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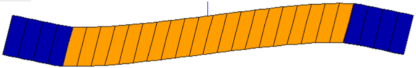

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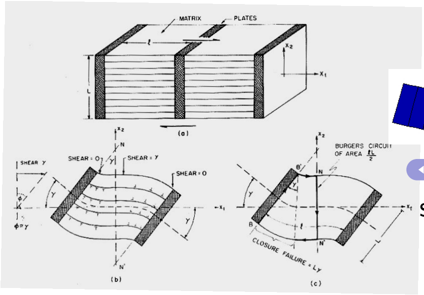

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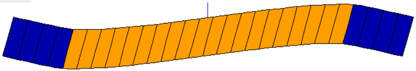

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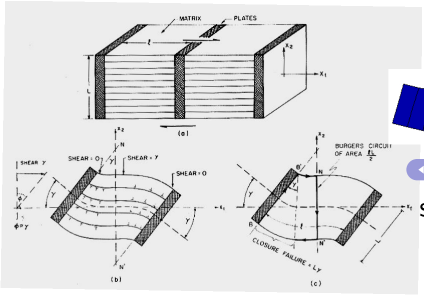

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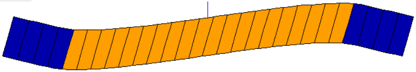

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Plan

Multiscale asymptotic expansions for heterogeneous Cosserat media

- macroscopic scale variable $\underline{\mathbf{x}}$, zoom at $\underline{\mathbf{y}} = \underline{\mathbf{x}}/\varepsilon$
- involved length scales: $\varepsilon = l/L_\omega$, l_c
- asymptotic expansions

$$\underline{\mathbf{u}}^{\varepsilon}(\underline{\mathbf{x}}) = \underline{\mathbf{u}}^{0}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \varepsilon\,\underline{\mathbf{u}}^{1}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \varepsilon^2\,\underline{\mathbf{u}}^{2}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \ldots$$

$$\underline{\mathbf{\Phi}}^{\varepsilon}(\underline{\mathbf{x}}) = \underline{\mathbf{\Phi}}^{0}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \varepsilon\,\underline{\mathbf{\Phi}}^{1}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \varepsilon^2\,\underline{\mathbf{\Phi}}^{2}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \ldots$$

$$\underset{\sim}{\boldsymbol{\sigma}}^{\varepsilon}(\underline{\mathbf{x}}) = \underset{\sim}{\boldsymbol{\sigma}}^{0}(\underline{\mathbf{x}},y) + \varepsilon\,\underset{\sim}{\boldsymbol{\sigma}}^{1}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \varepsilon^2\,\underset{\sim}{\boldsymbol{\sigma}}^{2}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \ldots$$

$$\underset{\sim}{\mathbf{m}}^{\varepsilon}(\underline{\mathbf{x}}) = \underset{\sim}{\mathbf{m}}^{0}(\underline{\mathbf{x}},y) + \varepsilon\,\underset{\sim}{\mathbf{m}}^{1}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \varepsilon^2\,\underset{\sim}{\mathbf{m}}^{2}(\underline{\mathbf{x}},\underline{\mathbf{y}}) + \ldots$$

Effective balance equations

- Case 1: Cosserat $\Longrightarrow$ Cauchy

$$\underset{\sim}{\boldsymbol{\sigma}}^{\varepsilon} = \underset{\approx}{\mathbf{C}}(\underline{\mathbf{y}}) : \underset{\sim}{\mathbf{e}}^{\varepsilon}(\underline{\mathbf{y}}), \quad \underset{\sim}{\mathbf{m}}^{\varepsilon} = \varepsilon^{2}\underset{\approx}{\mathbf{D}}(\underline{\mathbf{y}}) : \underset{\sim}{\boldsymbol{\kappa}}^{\varepsilon}(\underline{\mathbf{y}})$$

$$\begin{aligned} < \underset{\sim}{\boldsymbol{\sigma}}^{0} > .\boldsymbol{\nabla}_{x} + \underline{\mathbf{f}} &= 0 \\ -\underset{\approx}{\boldsymbol{\epsilon}} :< \underset{\sim}{\boldsymbol{\sigma}}^{0} > + \underline{\mathbf{c}} &= 0 \end{aligned}$$

- Case 2: Cosserat $\Longrightarrow$ Cosserat

$$\underset{\sim}{\boldsymbol{\sigma}}^{\varepsilon} = \underset{\approx}{\mathbf{C}}(\underline{\mathbf{y}}) : \underset{\sim}{\mathbf{e}}^{\varepsilon}(\underline{\mathbf{y}}) \quad \text{et} \quad \underset{\sim}{\mathbf{m}}^{\varepsilon} = \underset{\approx}{\mathbf{D}}(\underline{\mathbf{y}}) : \underset{\sim}{\boldsymbol{\kappa}}^{\varepsilon}(\underline{\mathbf{y}})$$

$$\begin{aligned} < \underset{\sim}{\boldsymbol{\sigma}}^{0} > .\boldsymbol{\nabla}_{x} + \underline{\mathbf{f}} &= 0 \\ < \underset{\sim}{\mathbf{m}}^{0} > .\boldsymbol{\nabla}_{x} - \underset{\approx}{\boldsymbol{\epsilon}} :< \underset{\sim}{\boldsymbol{\sigma}}^{0} > + \underline{\mathbf{c}} &= 0 \end{aligned}$$

Auxiliary problem on the unit cell

- periodic fluctuation

$$\underline{\mathbf{u}} = \underset{\sim}{\mathbf{E}}.\underline{\mathbf{y}} + \underline{\mathbf{v}}\,, \qquad \underline{\mathbf{\Phi}} = \underset{\sim}{\mathbf{K}}.\underline{\mathbf{y}} + \underline{\psi}, \quad \forall \underline{\mathbf{y}} \in V$$

- balance and constitutive equations

$$\underset{\sim}{\boldsymbol{\sigma}}.\boldsymbol{\nabla}_y = 0, \quad \underset{\sim}{\mathbf{m}}.\boldsymbol{\nabla}_y = 0$$

$$\underset{\sim}{\boldsymbol{\sigma}} = \underset{\approx}{\mathbf{C}} : (\underline{\mathbf{u}} \otimes \boldsymbol{\nabla}_y), \quad \underset{\sim}{\mathbf{m}} = \underset{\approx}{\mathbf{D}} : (\underline{\mathbf{\Phi}} \otimes \boldsymbol{\nabla}_y)$$

- Hill-Mandel's condition

$$< \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{e}} + \underset{\sim}{\mathbf{m}} : \underset{\sim}{\boldsymbol{\kappa}} >= \underset{\sim}{\mathbf{\Sigma}} : \underset{\sim}{\mathbf{E}} + \underset{\sim}{\mathbf{M}} : \underset{\sim}{\mathbf{E}}$$

where

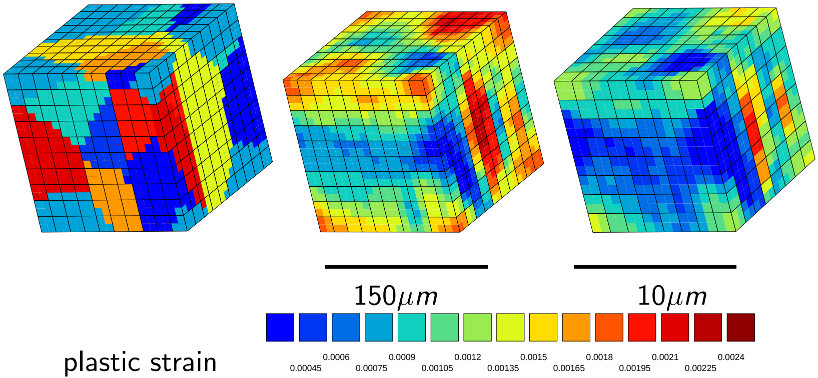
$$< \underline{\mathbf{u}} \otimes \boldsymbol{\nabla}_y >= \underset{\sim}{\mathbf{E}}, \quad < \underline{\mathbf{\Phi}} \otimes \boldsymbol{\nabla}_y >= \underset{\sim}{\mathbf{K}}$$

$$\underset{\sim}{\mathbf{\Sigma}} =< \underset{\sim}{\boldsymbol{\sigma}} >, \qquad \underset{\sim}{\mathbf{M}} =< \underset{\sim}{\mathbf{m}} >$$

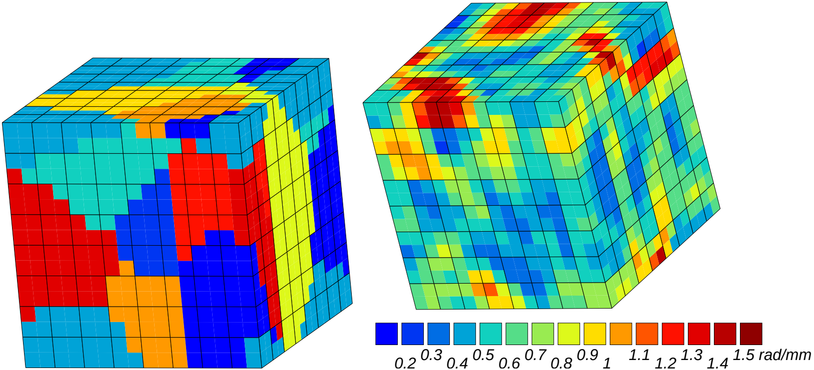
Plan

1. Representative volume element sizes for polycrystals
   - Bulk copper
   - Copper thin sheets
   - Equiaxial vs. pancake grains in zinc coatings
2. Grain size effect in polycrystals
   - Cosserat single crystal plasticity
   - Homogenization of Cosserat media
   - Hall–Petch effect in ferritic steels
3. Conclusions

Grain size effects in polycrystals



Lattice curvature in a ferritic steel



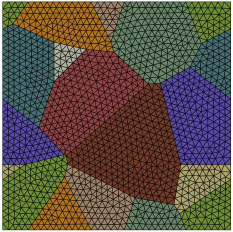
$\simeq 1 - 10^\circ/\mu m$

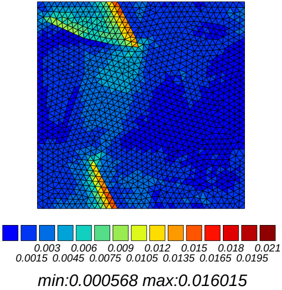
additional hardening $R^s(\theta^s) = Q_c \sqrt{\sum_r |\theta^r|}$

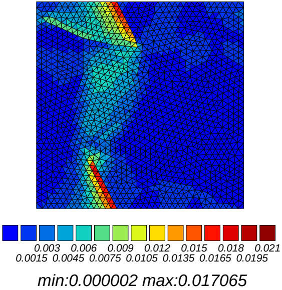
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: plastic strain





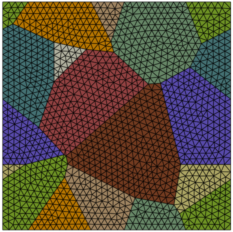


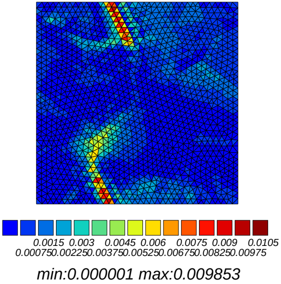
$150 \mu m$ $10 \mu m$

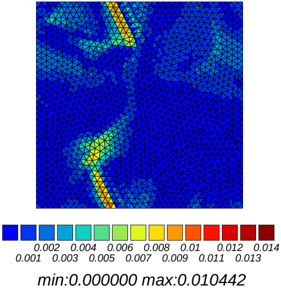
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: lattice rotation





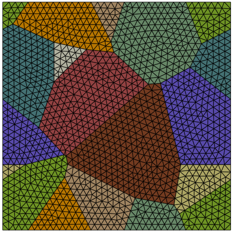


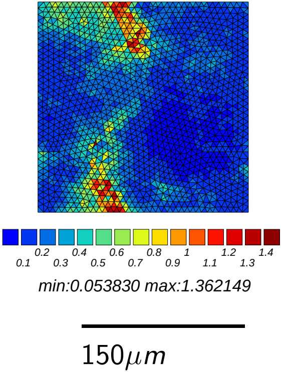
$150 \mu m$ $10 \mu m$

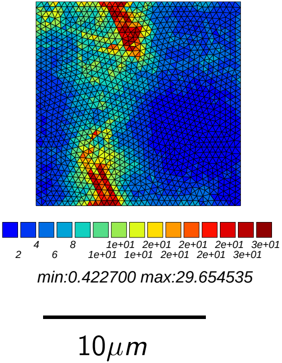
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity: lattice curvature



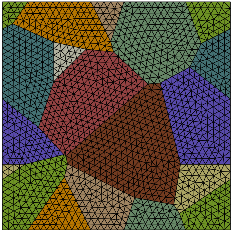


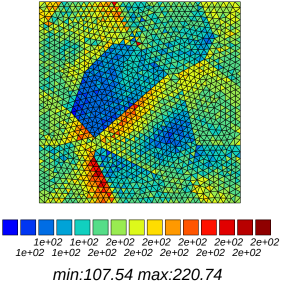


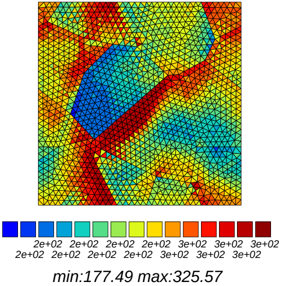
[Zeghadi, 2004]

Grain size effect in a ferritic steel

Microplasticity : local stresses





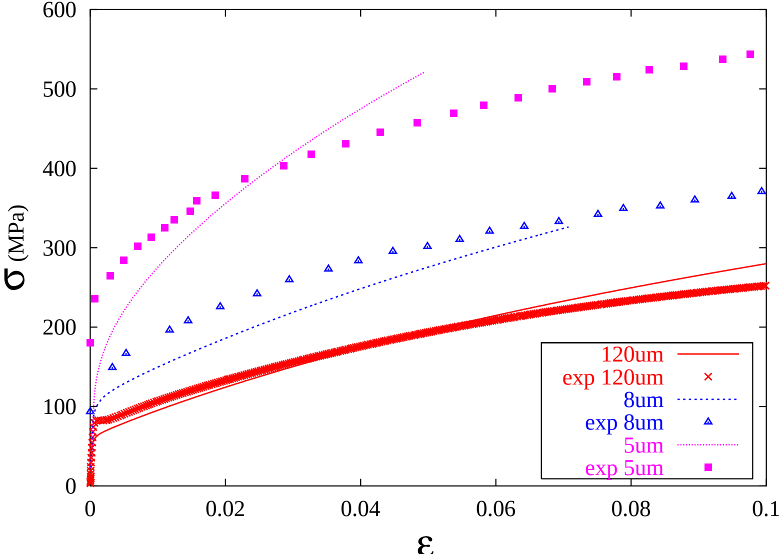


$150 \mu m$ $\qquad$ $10 \mu m$

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

[Zeghadi, 2004]

Grain size effects in a ferritic steel



[Bouaziz, 2002]

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Conclusions and prospects

- Cosserat crystals: an old story (Kröner, Mura...)
- Alternative continuum models for dislocated crystals

continuum	advantages	drawbacks	continuity
Cosserat	*easy implementation*	*skew–symmetric part?*	$\underline{\phi}$
second grade	*non geometrical effects*	*phenomenological* γ^S	$D_n \underline{\mathbf{u}}$
gradient of internal variable	*scalar*	*number of DOF*	γ^p
homogenization discrete/cont.	*rigorous*	*generality mathematical structure*	ρ^+, ρ^-

- quantitative predictions: additional hardening laws...
- other applications: crack tip plasticity, precipitate or particle hardening