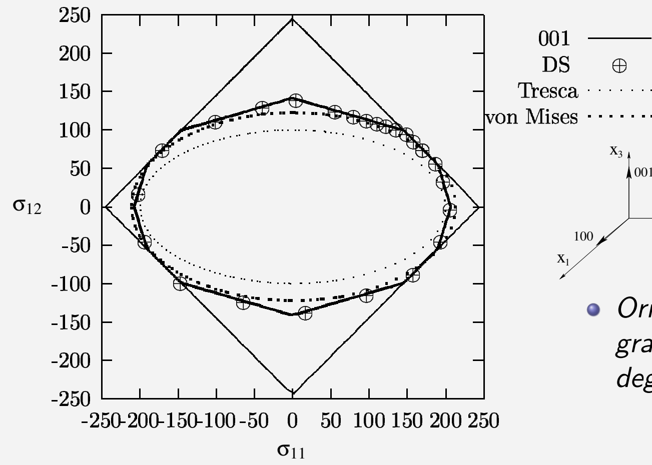
Contents

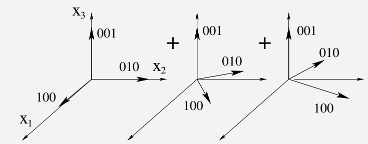
From single crystal to polycrystal
- Initial yield surfaces for DS material
- Initial yield surfaces for a polycrystalline material

Scale transition rules
- Various rules and their physical meaning

Main features of the polycrystal models
- Subsequent yield surfaces
- Complex paths
- Examples of FE computations using crystal plasticity
- Twinning and phase transformation

Yield surface for DS material with *3 orientations*





- *Orientations of the grains: 0, 30, 60 degrees*

More slip directions in the plane σ_{11}–σ_{12}: the model turns out to become similar to von Mises/Tresca

Use of uniform field models in Crystal plasticity

Georges Cailletaud

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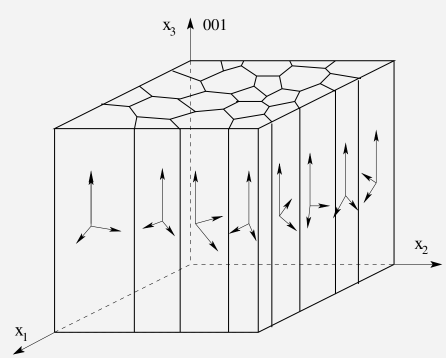
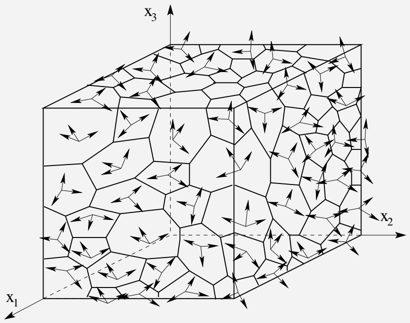
Ecole des Mines de Paris/CNRS

Loading surface of a directionally solidified material (DS)



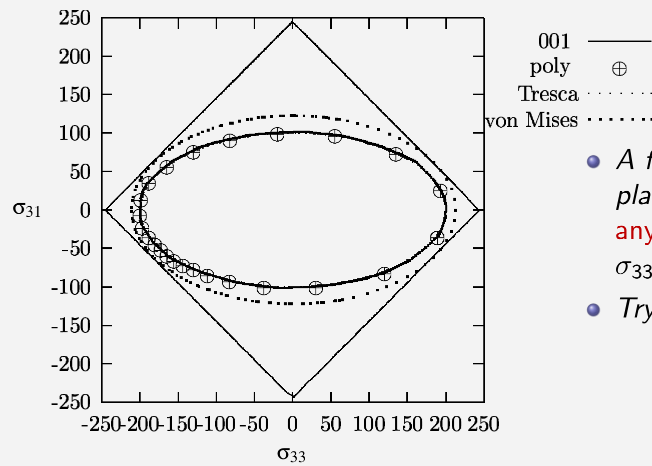
- *For a DS material, all the grains have a common crystal axis, say (001). The orientation of each grain is then defined by one angle around this axis.*
- *Assuming that elasticity is uniform, the stress is also uniform during the elastic phase.*

Loading surface of a polycrystalline material



- *The orientation of a grain is defined by a set of three Euler angles, (ϕ_1, Φ, ϕ_2)*
- *Assume an uniform elasticity*

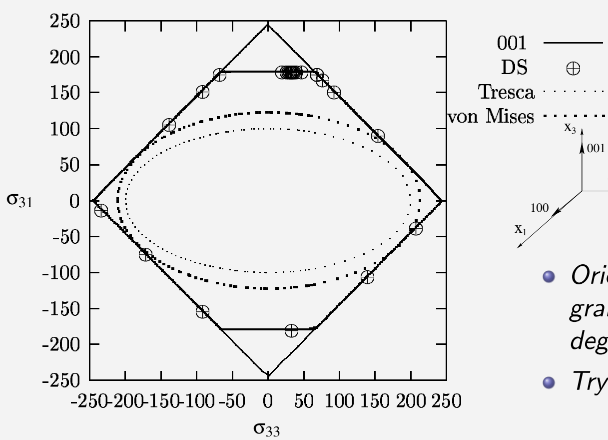
Yield surface for a polycristalline aggregate with *100 orientations*

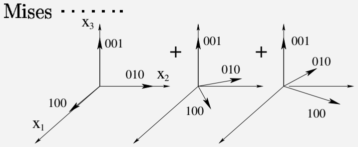


- *A favourably oriented plane can be found for any direction in the σ_{33}–σ_{31} plane*
- *Try an other set* HERE

Tresca like criterion is obtained for plane σ_{33}–σ_{31}

Yield surface for DS material with *3 orientations*

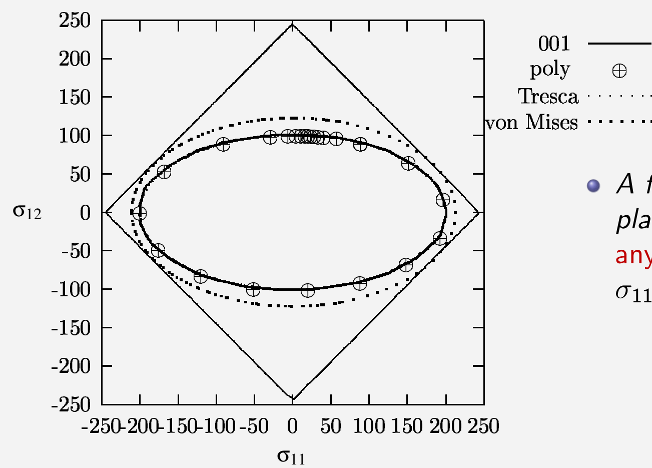




- *Orientations of the grains: 0, 30, 60 degrees*
- *Try an other set* HERE

No additional slip activated by shear in the plane σ_{33}–σ_{13}: the yield stress in shear remains high, and sharp corners are still present

Yield surface for a polycristalline aggregate with *100 orientations*

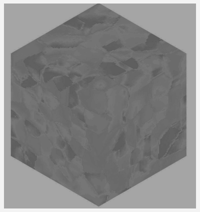


- *A favourably oriented plane can be found for any direction in the σ_{11}–σ_{12} plane*

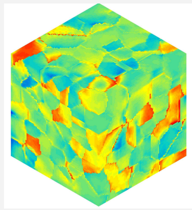
Tresca like criterion is obtained for plane σ_{11}–σ_{12}

Computations at various scales

Black box



Realistic aggregate



Intermediate level
Averaging
process
(2) phase by phase
(2') grain by grain

Level (1)	Level (3)	Level (2) or (2')
Macroscopic models	*Local information*	*Local average*
Average stress and strain tensor	*Respect local*	*Respect local*
	Constitutive Equations	*Constitutive Equations*
	Equilibrium	*no neighboring effect*
	Lectures 4 & 5	This lecture

Rules used for the scale transition in uniform field models

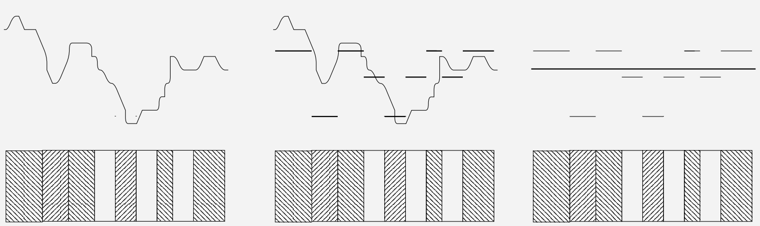
- *Static*, uniform stress, $\underset{\sim}{\sigma}^g = \underset{\sim}{\sigma}$
- *From Taylor to Kröner*
  - Taylor *[Taylor, 1938]*, uniform plastic strain, $\underset{\sim}{\varepsilon}^{pg} = \underset{\sim}{\varepsilon}^p$
  - Lin–Taylor *[Lin, 1957]*, uniform total strain, $\underset{\sim}{\varepsilon}^g = \underset{\sim}{\varepsilon}$
  - Kröner *[Kröner, 1971]*, elastic accommodation $\underset{\sim}{\sigma}^g = \underset{\sim}{\sigma} + \mu(\underset{\sim}{\varepsilon}^p - \underset{\sim}{\varepsilon}^{pg})$
- *Tangent and secant approximations*
  - Hill *[Hill, 1965]*, elastoplastic accommodation
    $\dot{\underset{\sim}{\sigma}}^g = \dot{\underset{\sim}{\sigma}} + \underset{\approx}{\mathbf{L}}^\star : (\dot{\underset{\sim}{\varepsilon}} - \dot{\underset{\sim}{\varepsilon}}^g)$
  - Berveiller–Zaoui *[Berveiller and Zaoui, 1979] estimation, with α varying typically between 1 and 0.001 (isotropic elasticity, spherical inclusions)* $\underset{\sim}{\sigma}^g = \underset{\sim}{\sigma} + \mu\alpha(\underset{\sim}{\varepsilon}^p - \underset{\sim}{\varepsilon}^{pg})$
- *Viscous and viscoplastic scheme*
  - Budianski, Hutchinson, Molinari,... *[Hutchinson, 1966a, Molinari et al., 1987a]*
  - Translated fields *[Sabar et al., 2002]*,
    $\dot{\underset{\sim}{\sigma}}^g = \dot{\underset{\sim}{\sigma}} + 2\mu(1-\beta)(\frac{5\eta}{3\eta + 2\eta^g}\dot{\underset{\sim}{\varepsilon}}^v - \dot{\underset{\sim}{\varepsilon}}^{vg})$
- *Parametric scale transition rule*
  - Cailletaud, Pilvin , β–model

Various scales in heterogeneous material modeling

(a) *Microstructure calculations: take into account local phases and local equilibrium (*Next two lectures *)*

(b) *Uniform field models: take into account local phases only (*This lecture *)*

(c) *Macroscopic models: do not account for local phases nor local equilibrium*

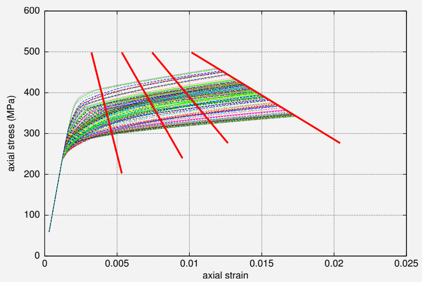


(a) (b) (c)

Definitions used in the transition rules

- *Phase characteristics*
  - *Chemical composition, shape, crystallographic orientation*
  - *f^g is the volume fraction of the phase g*
  - *The choice of the* representation *of a phase is driven by the contrast between properties. Two phase polycristal→ two phases, discriminating by the chemical nature, or the crystal network; one phase polycristal→ N crystallographic phases*
- *Notations:*
  - *Stress in the phase g, macroscopic stress:* $\underset{\sim}{\sigma}^g$, $\underset{\sim}{\sigma} = \sum_g f^g \underset{\sim}{\sigma}^g$
  - *Strain in the phase g, macroscopic strain:* $\underset{\sim}{\varepsilon}^g$, $\underset{\sim}{\varepsilon} = \sum_g f^g \underset{\sim}{\varepsilon}^g$
  - *For an uniform local elasticity, the macroscopic plastic strain is also the average of the local plastic strains:* $\underset{\sim}{\varepsilon}^p = \sum_g f^g \underset{\sim}{\varepsilon}^{pg}$

Physical meaning of Berveiller–Zaoui rule



- *Uniform elasticity*
- *Incompressible plastic flow*
- *Radial loading path*
- *General expression, using μ', actual shear modulus, $\beta' = 2(4-5\nu')/15(1-\nu')$*

$$\dot{\underset{\sim}{\sigma}}^g = \dot{\underset{\sim}{\sigma}} + 2\mu\frac{\mu'(1-\beta')}{\beta'\mu+(1-\beta')\mu'}(\dot{\underset{\sim}{\varepsilon}}^p - \dot{\underset{\sim}{\varepsilon}}^{pg})$$

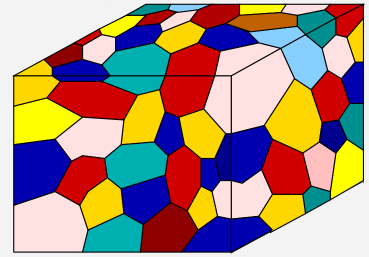
- *Pure tension, assuming $\nu = 1/2$ and introducing $H = \sigma/\varepsilon^p$:*

$$\dot{\sigma}_g = \dot{\sigma} + \frac{\mu H}{H+2\mu}(\dot{\varepsilon}^p - \dot{\varepsilon}^{pg})$$

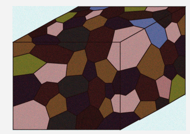
- *Onset of plastic flow: Kröner's rule*
- *The accommodation factor $C = (\sigma^g - \sigma)/(\varepsilon^p - \varepsilon^{pg})$ decreases when plastic strain increases*

Calibration of the scale transition rule

- *FE computation*

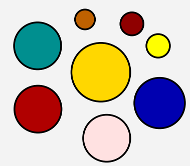


- *Global response*



$\underset{\sim}{\sigma}$
$\underset{\sim}{\varepsilon}$

- *Local response*

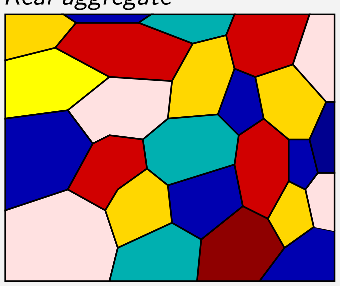


$\underset{\sim}{\sigma}^g$
$\underset{\sim}{\varepsilon}^g$

1. *Perform a FE computation of a realistic aggregate*
2. *Post-treatment to get the macroscopic stress and strain*
3. *Post-treament to get the average values in each phase*
4. *Identification of the parameters of the transition rule to have a good fit for both global and local levels*

Hill's self–consistent model

- *Real aggregate*



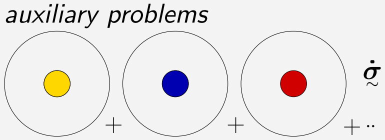
$$\dot{\underset{\sim}{\sigma}} = \dot{\underset{\sim}{\Sigma}} + \underset{\approx}{L}^\star : (\dot{\underset{\sim}{E}} - \dot{\underset{\sim}{\varepsilon}})$$

with $\underset{\approx}{L}^\star$, accommodation tensor:

$$\underset{\approx}{L}^\star = \underset{\approx}{L}^{\text{eff}} : (\underset{\approx}{S}^{-1} - \underset{\approx}{I})$$

$$(\underset{\approx}{L} + \underset{\approx}{L}^\star) : \dot{\underset{\sim}{\varepsilon}} = (\underset{\approx}{L}^{\text{eff}} + \underset{\approx}{L}^\star) : \dot{\underset{\sim}{E}}$$

- *Modelled as a collection of auxiliary problems*



t

$$\dot{\underset{\sim}{\sigma}} = \underset{\approx}{L} : (\underset{\approx}{L} + \underset{\approx}{L}^\star)^{-1} : (\underset{\approx}{L}^{\text{eff}} + \underset{\approx}{L}^\star) : \dot{\underset{\sim}{E}}$$

So that :

$$\underset{\approx}{L}^{\text{eff}} = < \underset{\approx}{L} : (\underset{\approx}{L} + \underset{\approx}{L}^\star)^{-1} : (\underset{\approx}{L}^{\text{eff}} + \underset{\approx}{L}^\star) >$$

- *implicit problem, since the HEM is not known*

Introduction of a parametric scale transition rule

- *The local stress decrease when the grain becomes more plastic than the matrix*

$$\underset{\sim}{\sigma}^g = \underset{\sim}{\sigma} + C\left(\underset{\sim}{B} - \underset{\sim}{\beta}^g\right)$$

$$\underset{\sim}{B} = \sum_g f_g \underset{\sim}{\beta}^g$$

f_g is the volume fraction of phase g, $\underset{\sim}{\beta}^g$ characterizes the state of redistribution

- *New interphase accommodation variables $\underset{\sim}{\beta}^g$, with a kinematic evolution rule [Cailletaud 87]*

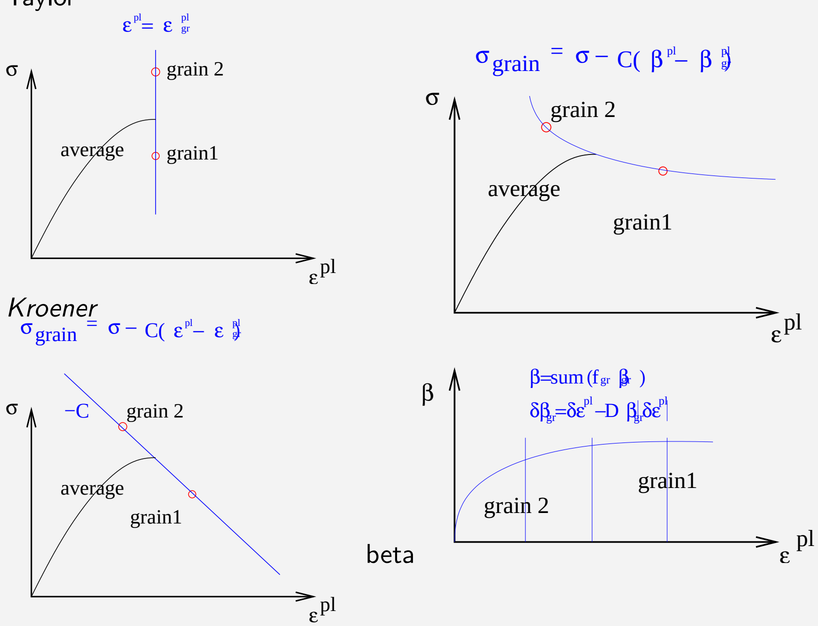
  - rule 1: $\dot{\underset{\sim}{\beta}}^g = \dot{\underset{\sim}{\varepsilon}}^g - D\dot{\varepsilon}^g_{eq}\underset{\sim}{\beta}^g$

  - rule 2: $\dot{\underset{\sim}{\beta}}^g = \dot{\underset{\sim}{\varepsilon}}^g - D\dot{\varepsilon}^g_{eq}(\underset{\sim}{\beta}^g - \delta\underset{\sim}{\varepsilon}^g)$

- *Identification procedure, inverse approach from finite element [Pilvin 97]: the coefficient C, D, δ, are not exactly material coefficients,* but scale transition parameters, *which should be fitted from Finite Element computation on realistic polycrystalline aggregates.*

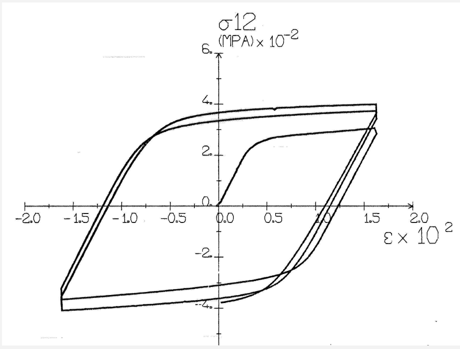
Summary of the scale transition rules

Taylor



Distorsion of a yield surface

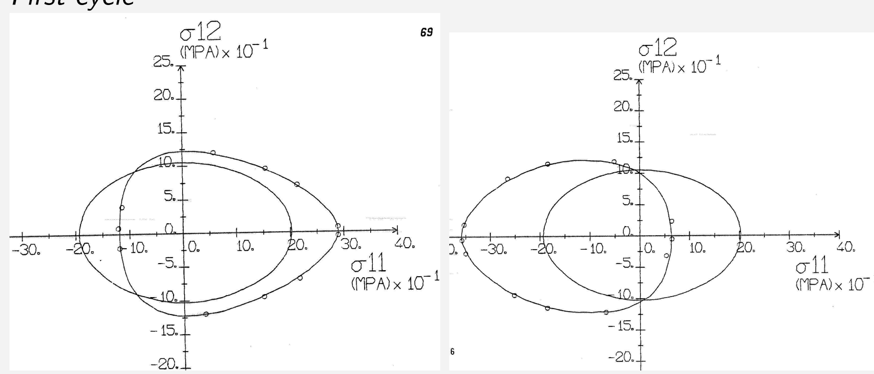
Fatigue tests on a 2024 aluminium alloy



PhD Marc Rousset, 1985

Experimental distorsion of a yield surface (1)

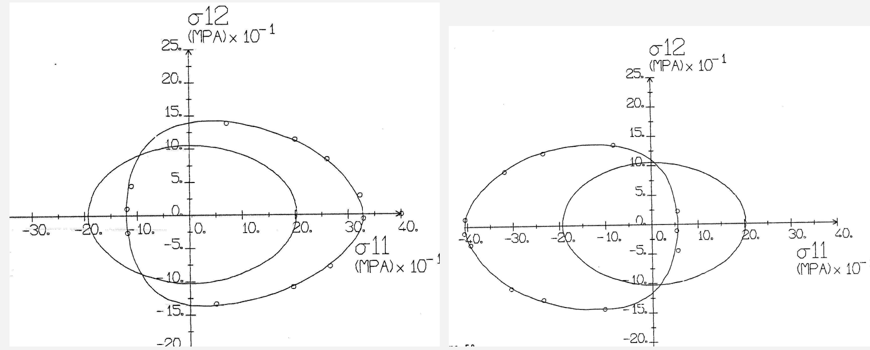
First cycle



PhD Marc Rousset, 1985

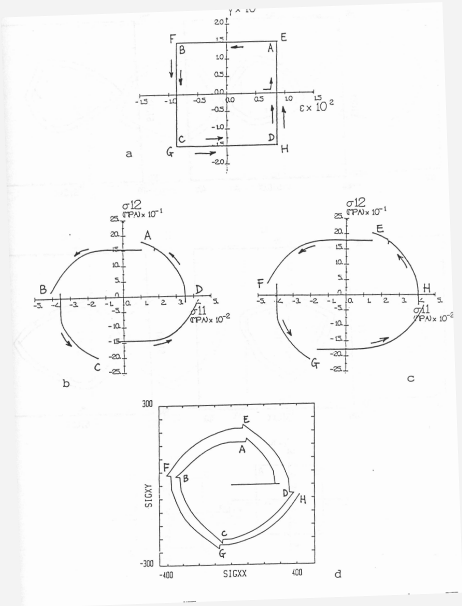
Experimental distorsion of a yield surface (1bis)

Second cycle



PhD Marc Rousset, 1985

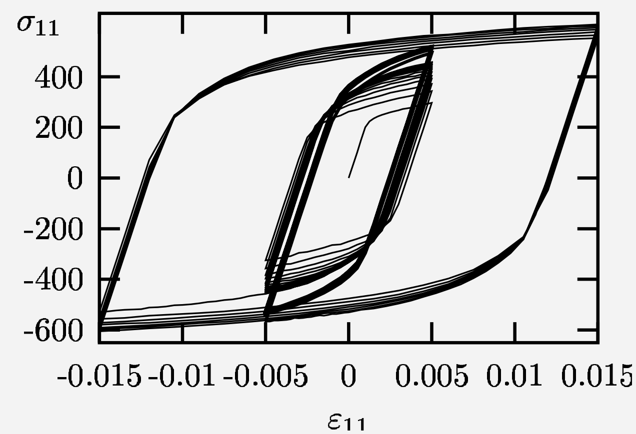
Experimental distorsion of a yield surface (2)



- *Square path in the ε_{11}–ε_{12} plane*
- *Yield surface investigation for each corner, at 1st and 2nd cycle*
- *Low viscous effect*
- *Good prediction of the stress response in the σ_{11}–σ_{12} plane*

PhD Marc Rousset, 1985

Simulation of the memory effect

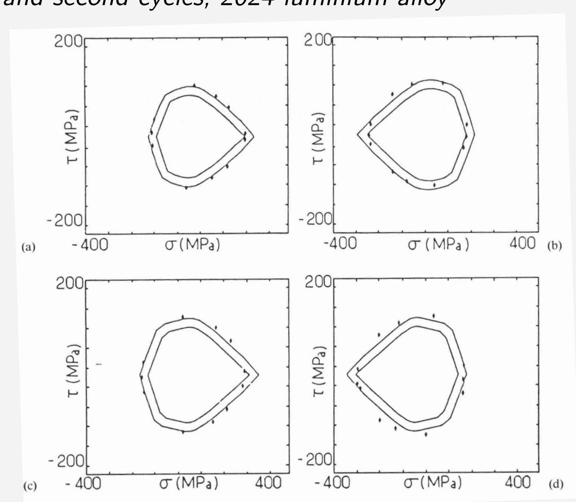


R_0	Q	b	c	d	h_i
100	50	10	5000	100	1, i

[Besson et al., 2001]

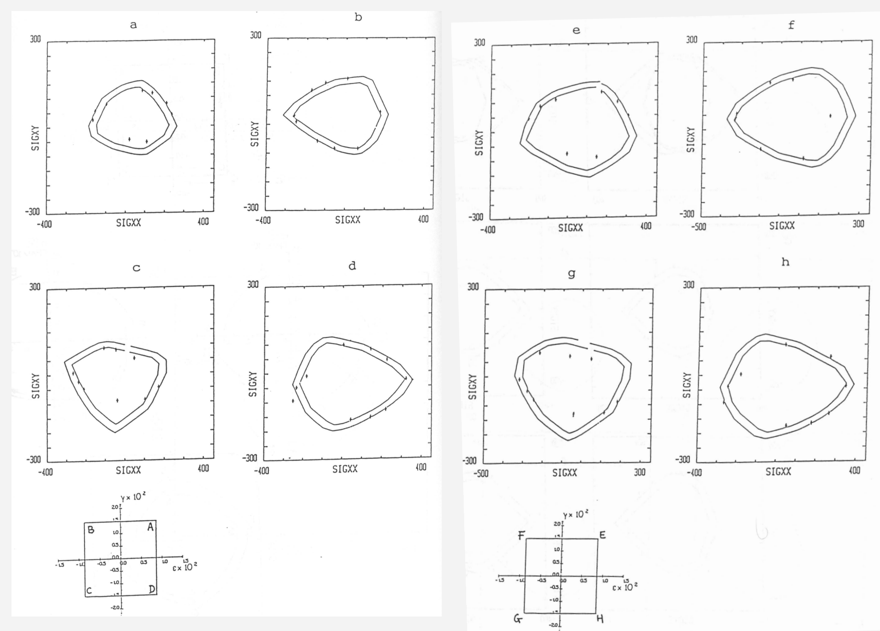
Simulation of the distorsion of a yield surface

First cycle and second cycles, 2024 luminium alloy



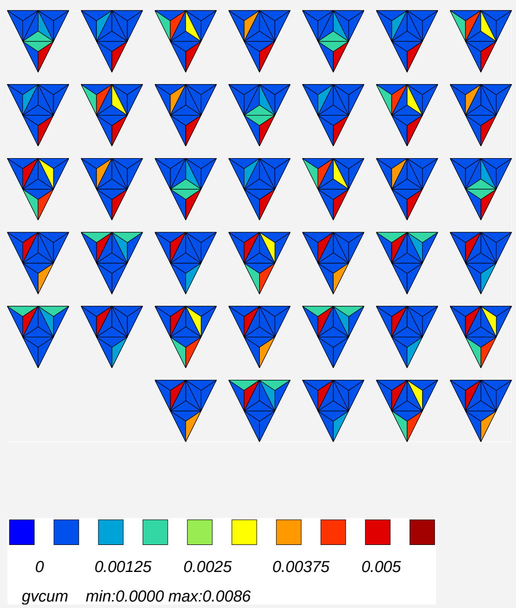
[Cailletaud, 1992]

Simulation of the distorsion of a yield surface



[Cailletaud, 1992]

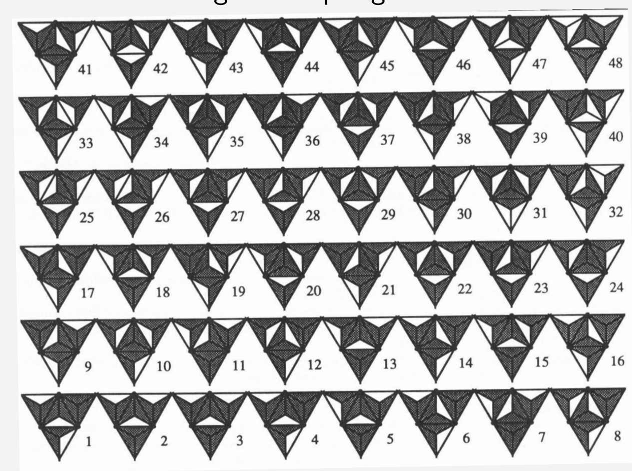
Contour of accumulated slip after a tension test



FCC grains, 12 slip systems are reported in each big triangles

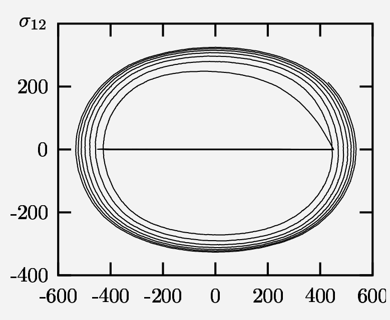
Active slip systems for an out-of-phase test

Average value per grain: 3.25

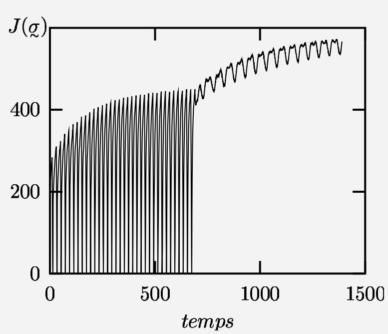


Simulation of the additional hardening obtained in out-of-phase tension-shear loading

The loading is a circle in ε_{11}–ε_{12} plane



Response in the stress plane

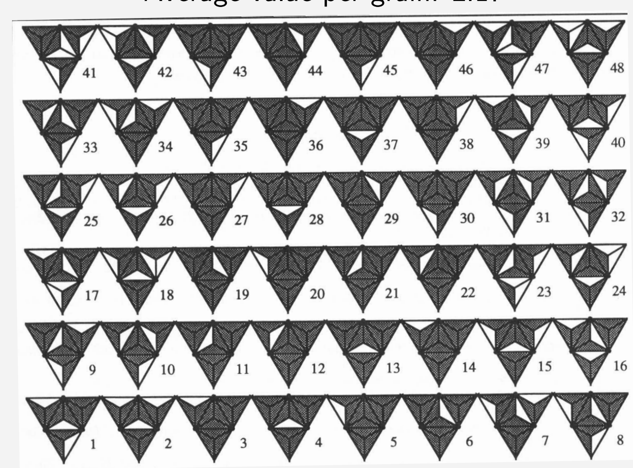


Evolution of the equivalent stress

[Besson et al., 2001]

Active slip systems in tension

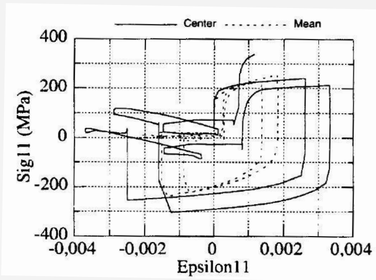
Average value per grain: 2.17



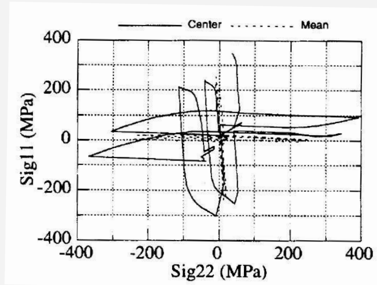
Active systems in white

A 3D specimen: computation results

A polycrystal models in each Gauss point

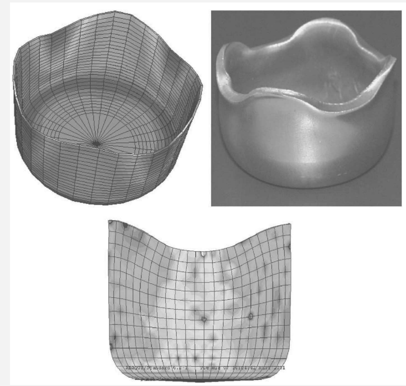


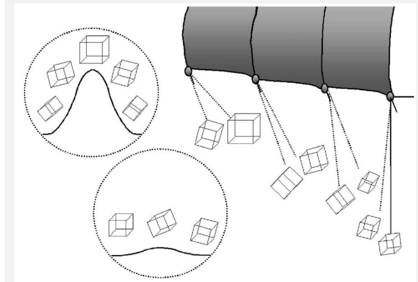
Hysteresis loop
for 11 component



Loading path in
the $\sigma_{11} - \sigma_{22}$ plane

Deep drawing, one polycristal for each Gauss point

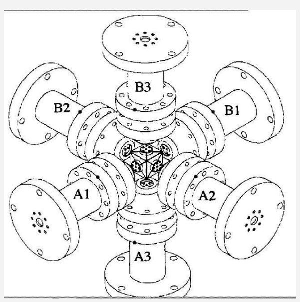




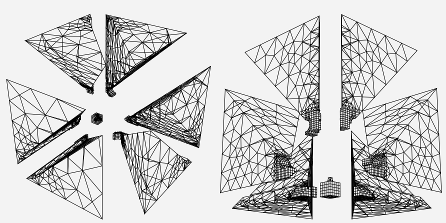
(more in [Raabe and Roters, 2004])

A 3D specimen (exp. made at LMT Cachan)

A polycrystal models in each Gauss point



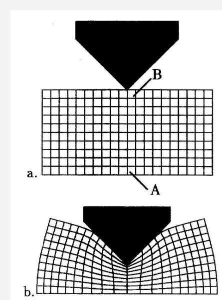
Schematic view
of the specimen



The mesh with
subdomains for parallel computation

(more in [Feyel et al., 1997])

Indentation, one polycristal for each Gauss point



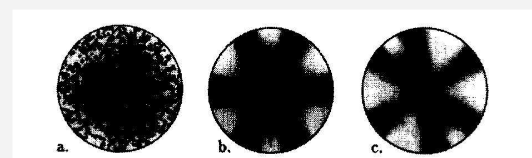


Fig. 26. Punch indentation problem. {111}-pole figures: (a) Initial orientation distribution; (b) texture development in point A; (c) texture development in point B.

(more in [Miehe et al., 1999])

Literature

- *Books and reviews* *[Dawson, 2000, Besson et al., 2001, Bornert et al., 2001]*
- *Polycrystal effect [Cailletaud, 1992, Sarma and Dawson, 1996, Dawson and Marin, 1998, Nemat-Nasser and Li, 1998]*
- *Scale transition rules [Hutchinson, 1966b, Berveiller and Zaoui, 1979, Molinari et al., 1987b, Pilvin and Cailletaud, 1990, Cailletaud and Pilvin, 1994, Forest and Pilvin, 1995, Sabar et al., 2002]*
- *Twining and phase transformation* *[Cherkaoui et al., 2000, Staroselski and Anand, 1998]*
- *Finite Element computations with polycrystals,* *[Feyel et al., 1997, Miehe et al., 1999, Raabe and Roters, 2004]*

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