

Multisurface models, crystal plasticity



- **General framework**
- **Models using von Mises type criteria**
- **Single crystal**
- **Multicrystal**
- **Polycrystal, the β -rule**

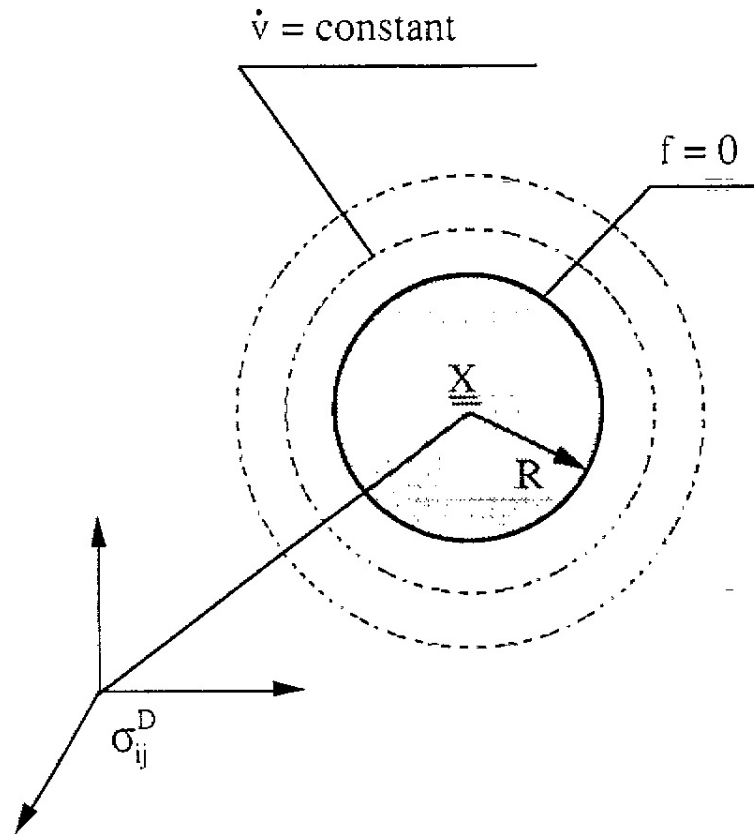
–Review alternative modeling routes–

Definition

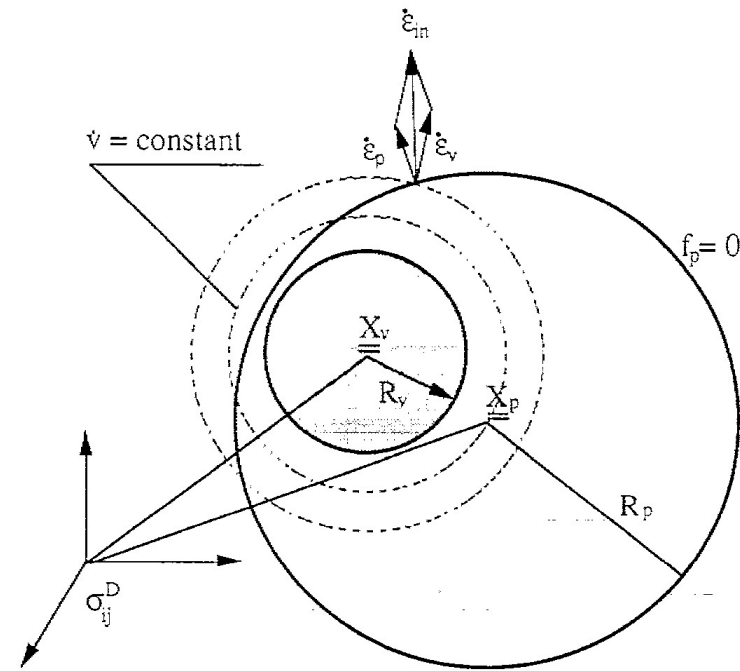
- Multisurface: several yield surfaces
- A *mechanism* is a set of isotropic and kinematic variables
- Several mechanisms can be involved in a yield surface
- Several mechanisms can be involved in several yield surfaces
- Possibility of coupling between mechanisms and surface evolution
- Other denomination: *multipotential*
- NB: surfaces for yielding, flow direction, hardening rules

First developed by Koiter (1960), Mandel (1965)

Multimechanism versus unified models (1)



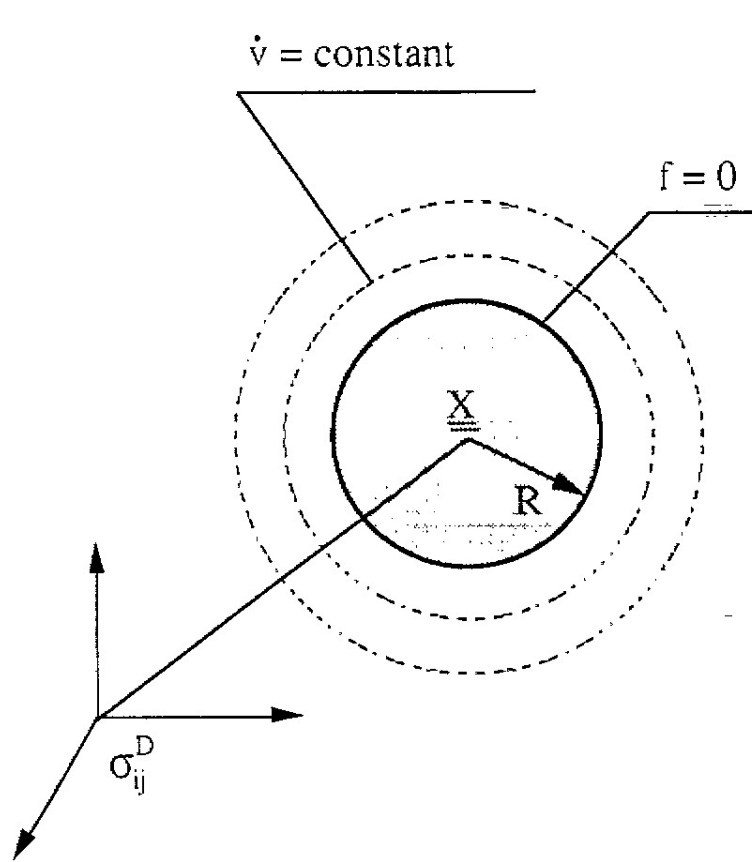
Unified model



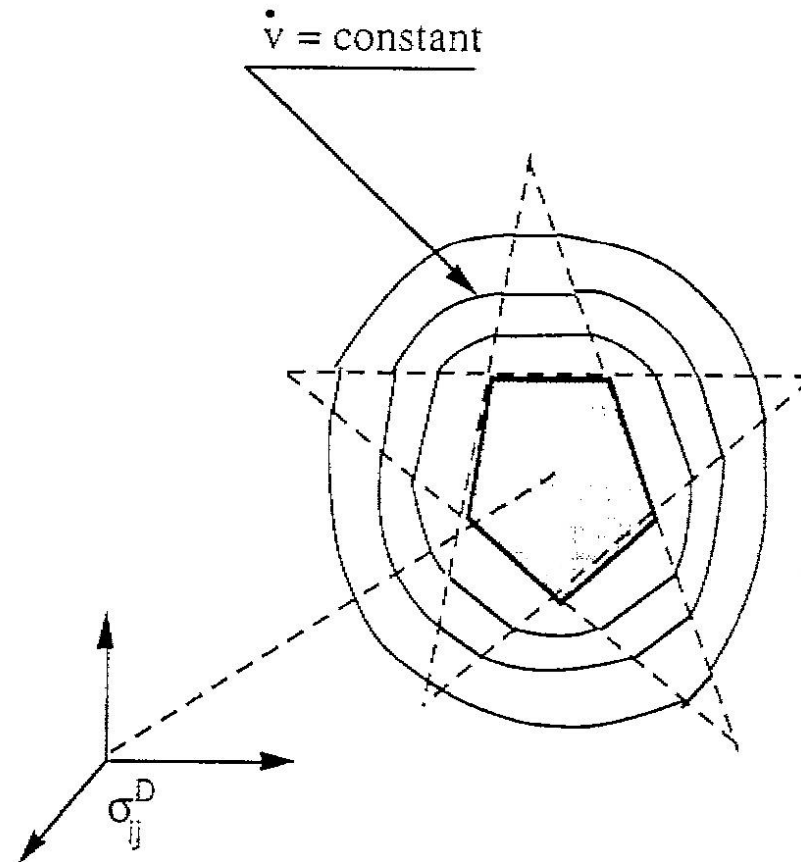
Multimechanism

Example of a multimechanism model with von Mises local criteria

Multimechanism versus unified models (2)



Unified model



Multimechanism

Example of a multimechanism model with linear local criteria

Anatomy of a multimechanism model

- Several sets of variables Z
- Free energy $\psi = \sum_s \psi_s(Z_{J_s}^s)$
- Elementary stress for each mechanism, $\underline{\sigma}^s$
 - ★ Stress concentration tensor, from global to local $\underline{\underline{B}}^s = \frac{\partial \underline{\sigma}^s}{\partial \underline{\sigma}}$
 - ★ Each $\underline{\sigma}^s$ is involved in a local criterion f^s , and: $\underline{\underline{n}}^s = \frac{\partial f^s}{\partial \underline{\sigma}^s}$
 - ★ Each $\underline{\sigma}^s$ is involved in a global criterion f , and: $\underline{\underline{n}}^s = \frac{\partial f}{\partial \underline{\sigma}^s}$

Each mechanism is either plastic or viscoplastic

Plastic flow for a multimechanism model

- Each $\underline{\sigma}^s$ is involved in a local criterion f^s

$$\underline{\dot{\epsilon}}^p = \sum_s \frac{\partial \Omega^s}{\partial \underline{\sigma}} = \sum_s \frac{\partial \Omega^s}{\partial f^s} \frac{\partial f^s}{\partial \underline{\sigma}} = \sum_s \frac{\partial \Omega^s}{\partial f^s} \underline{n}^s : \underline{B}^s$$

see later 2M2C model and crystal plasticity

- Each $\underline{\sigma}^s$ is involved in a global criterion f

$$\underline{\dot{\epsilon}}^p = \frac{\partial \Omega}{\partial \underline{\sigma}} = \frac{\partial \Omega}{\partial f} \frac{\partial f}{\partial \underline{\sigma}} = \frac{\partial \Omega}{\partial f} \sum_s \underline{n}^s : \underline{B}^s$$

see later 2M1C model

A few examples

- 2M2C: 2 mechanisms $(\underline{X}^1, R^1), (\underline{X}^2, R^2)$, two criteria (f^1, f^2)
- 2M1C: 2 mechanisms $(\underline{X}^1, R^1), (\underline{X}^2, R^2)$, one criterion (f)
- Single crystal: S mechanisms (x^s, r^s) , S criteria (f^s) ($S \equiv$ number of slip systems)
- Polycrystal: $S \times G$ mechanisms (x^s, r^s) , $S \times G$ criteria (f^s) ($G \equiv$ number of grains)
- Comments on the β -rule for heterogeneous materials

2M2C model: state variables and flow

Free energy:

$$\rho\psi = \frac{1}{3} \sum_I \sum_J C_{IJ} \underline{\alpha}^I : \underline{\alpha}^J$$

$$+ \frac{1}{2} \sum_I b_I Q_I (r^I)^2$$

$$\underline{\mathbf{X}}^I = \frac{2}{3} \sum_J C_{IJ} \underline{\alpha}^J$$

$$R^I = b_I Q_I r^I$$

Flow:

$$\Omega = \Omega^1(f^1) + \Omega^2(f^2)$$

$$f^I = J(\underline{\sigma} - \underline{\mathbf{X}}^I) - R^I - R_0^I$$

$$\underline{\dot{\epsilon}}^p = \frac{\partial \Omega^1}{\partial f^1} \underline{\mathbf{n}}^1 + \frac{\partial \Omega^2}{\partial f^2} \underline{\mathbf{n}}^2$$

$$\text{with } \underline{\mathbf{n}}^I = \frac{\partial f^I}{\partial \underline{\sigma}}$$

Each flow can be viscoplastic or plastic

2M2C model: hardening

Dissipation:

$$\dot{\tilde{\alpha}}^I = \left(\tilde{\mathbf{n}}^I - \frac{3D_I}{2C_{II}} \mathbf{X}^I \right) \frac{\partial \Omega^I}{\partial f^I}$$

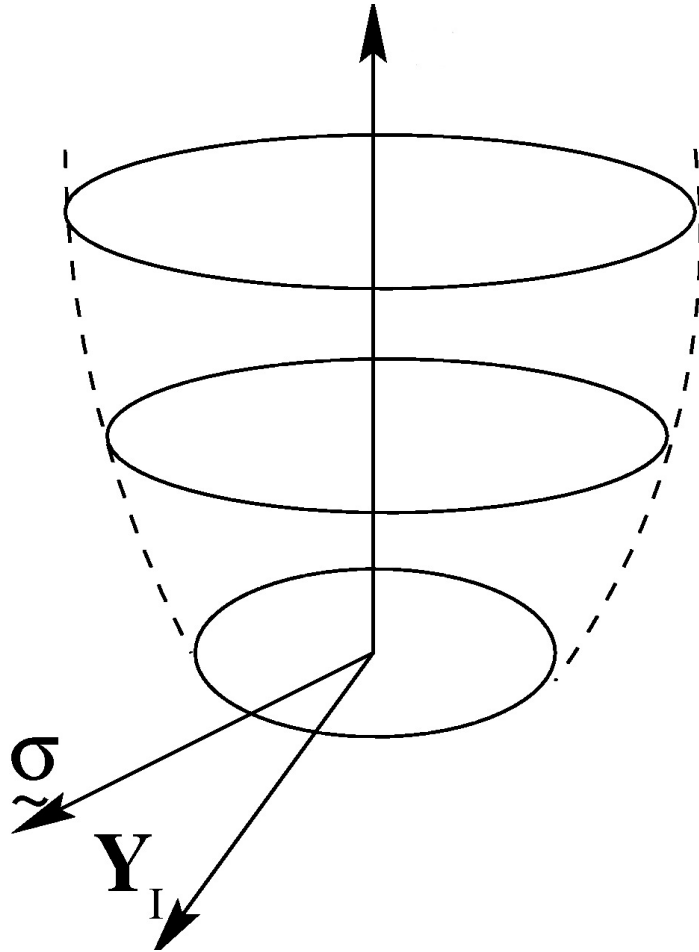
$$\dot{r} = \left(1 - \frac{R^I}{Q_I} \right) \frac{\partial \Omega^I}{\partial f^I}$$

- Denote $\dot{p}^I = \frac{\partial \Omega^I}{\partial f^I}$ for plastic flow
- Denote $\dot{v}^I = \frac{\partial \Omega^I}{\partial f^I}$ for viscoplastic flow

Three possible models:

- 2M2C-VV: $\dot{\tilde{\epsilon}}^p = \dot{v}^1 \tilde{\mathbf{n}}^1 + \dot{v}^2 \tilde{\mathbf{n}}^2$
- 2M2C-PP: $\dot{\tilde{\epsilon}}^p = \dot{p}^1 \tilde{\mathbf{n}}^1 + \dot{p}^2 \tilde{\mathbf{n}}^2$
- 2M2C-VP: $\dot{\tilde{\epsilon}}^p = \dot{v}^1 \tilde{\mathbf{n}}^1 + \dot{p}^2 \tilde{\mathbf{n}}^2$

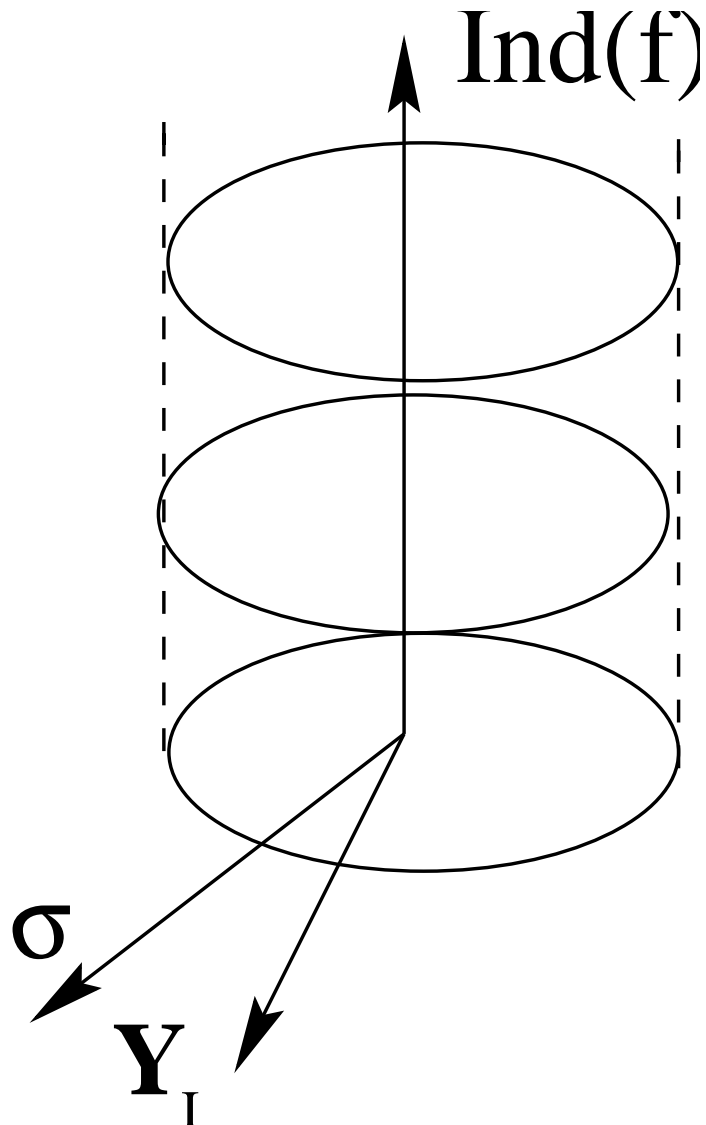
2M2C-VV model



\dot{v}^1 and \dot{v}^2 are directly defined from
 $\frac{\partial \Omega^1}{\partial f^1}$ and $\frac{\partial \Omega^2}{\partial f^2}$

For instance, $\dot{v}^I = \left(\frac{f^I}{K_I} \right)^{n_I}$

2M2C-PP model



\dot{p}^1 and \dot{p}^2 are defined from the consistency conditions $\dot{f}^1 = 0$ and $\dot{f}^2 = 0$

- no active mechanism
- one mechanism only
- two mechanisms

$$f^I = J(\underline{\sigma} - \underline{X}^I) - R^I - R_O^I$$

$$\dot{f}^I = \underline{n}^I : \underline{\dot{\sigma}} - \underline{n}^I \underline{\dot{X}}^I - \dot{R}^I$$

Coupling through:

$$\underline{\dot{X}}^I = C_{II} \dot{\alpha}^{II} + C_{IJ} \dot{\alpha}^{IJ}$$

2M2C-PP model (2)

For two mechanisms:

$$\dot{\lambda}^1 = \left\langle \frac{M_{22} \tilde{\mathbf{n}}^1 : \dot{\tilde{\boldsymbol{\sigma}}} - M_{12} \tilde{\mathbf{n}}^2 : \dot{\tilde{\boldsymbol{\sigma}}}}{M_{11} M_{22} - M_{12} M_{21}} \right\rangle$$

$$\dot{\lambda}^2 = \left\langle \frac{M_{11} \tilde{\mathbf{n}}^2 : \dot{\tilde{\boldsymbol{\sigma}}} - M_{21} \tilde{\mathbf{n}}^1 : \dot{\tilde{\boldsymbol{\sigma}}}}{M_{11} M_{22} - M_{12} M_{21}} \right\rangle$$

with

$$M_{II} = C_{II} - D_I \tilde{\mathbf{X}}^I : \tilde{\mathbf{n}}^I + b_I (Q_I - R^I)$$

$$M_{IJ} = \frac{2}{3} C_{IJ} \tilde{\mathbf{n}}^I : \tilde{\mathbf{n}}^J - D_J \frac{C_{IJ}}{C_{JJ}} \tilde{\mathbf{n}}^I : \tilde{\mathbf{X}}^J$$

2M2C-VP model

$$\begin{aligned}
 f^v &= J(\underline{\sigma} - \underline{X}^v) - R^v - R_{ov} & f^p &= J(\underline{\sigma} - \underline{X}^p) - R^p - R_{op} \\
 \underline{X}^v &= (2/3)C_v \underline{\alpha}^v + C_{vp} \underline{\alpha}^p & \underline{X}^p &= (2/3)C_p \underline{\alpha}^p + C_{vp} \underline{\alpha}^v \\
 R^v &= b_v Q_v r^v & R^p &= b_p Q_p r^p \\
 \dot{\underline{\alpha}}^v &= \dot{\underline{\varepsilon}}^v - \left(\frac{3D_v}{2C_v} \right) \underline{X}^v \dot{v} & \dot{\underline{\alpha}}^p &= \dot{\underline{\varepsilon}}^p - \left(\frac{3D_p}{2C_p} \right) \underline{X}^p \dot{\lambda} \\
 \dot{r}^v &= \left(1 - \frac{R^v}{Q_v} \right) \dot{v} & \dot{r}^p &= \left(1 - \frac{R^p}{Q_p} \right) \dot{p} \\
 \dot{\lambda} &= \frac{\langle \dot{\underline{\sigma}} - C_{vp} \dot{\underline{\alpha}}^v \rangle : \underline{n}^p}{H_p} & \text{with } H_p &= C_p - D_p \underline{X}^p : \underline{n}^p + b_p (Q_p - R^p) \\
 \dot{v} &= \left\langle \frac{f^v}{K} \right\rangle^n
 \end{aligned}$$

2M2C-VP model(2)

Note on the consistency condition for 2M2C-VP model:

$$\dot{f}^p = \underline{\underline{n}}^p : \underline{\underline{\dot{\sigma}}} - \underline{\underline{n}}^p \underline{\underline{\dot{X}}}^p - \dot{R}^p$$

Coupling through:

$$\underline{\underline{\dot{X}}}^p = C_{pp} \underline{\underline{\dot{\alpha}}}^{pp} + C_{vp} \underline{\underline{\dot{\alpha}}}^{vp}$$

$$\underline{\underline{\dot{X}}}^p = C_{pp} \left(\underline{\underline{n}}^p - \frac{3D_p}{2C_{pp}} \underline{\underline{X}}^p \right) \dot{p} + C_{vp} \left(\underline{\underline{n}}^v - \frac{3D_v}{2C_{vv}} \underline{\underline{X}}^v \right) \dot{v}$$

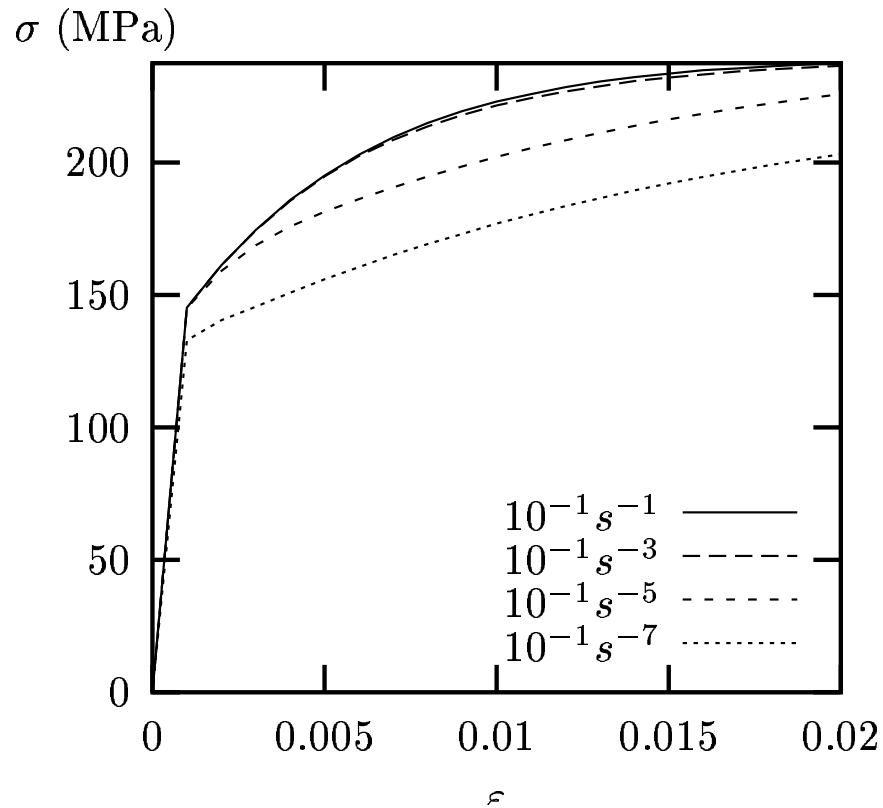
$$\dot{R}^p = b_p Q_p \left(1 - \frac{R^p}{Q_p} \right) \dot{p}$$

\dot{p} becomes time dependent...

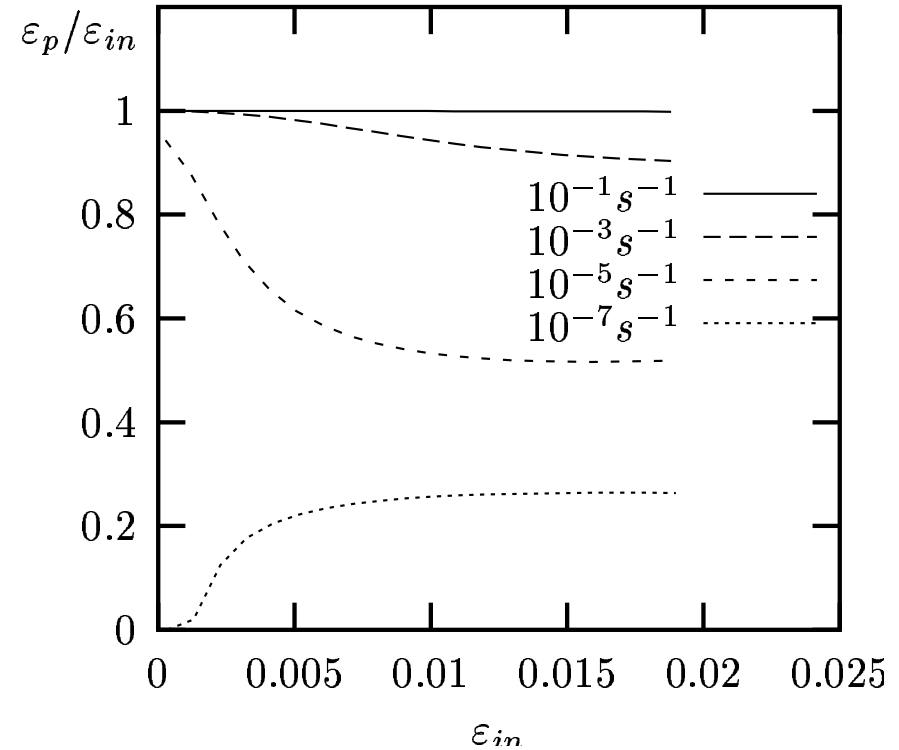
2M2C-VP model(2)

- Limitation of the viscous stress for very high strain rate by the time independent model
- The yield limit for creep can be much lower than yield limit for inviscid plasticity
- Full/limited coupling between plasticity and creep
- Special coefficient sets provide *inverse strain rate* effect (lower stress for higher strain rate)

2M2C-VP model: Balance between plastic and viscoplastic strain



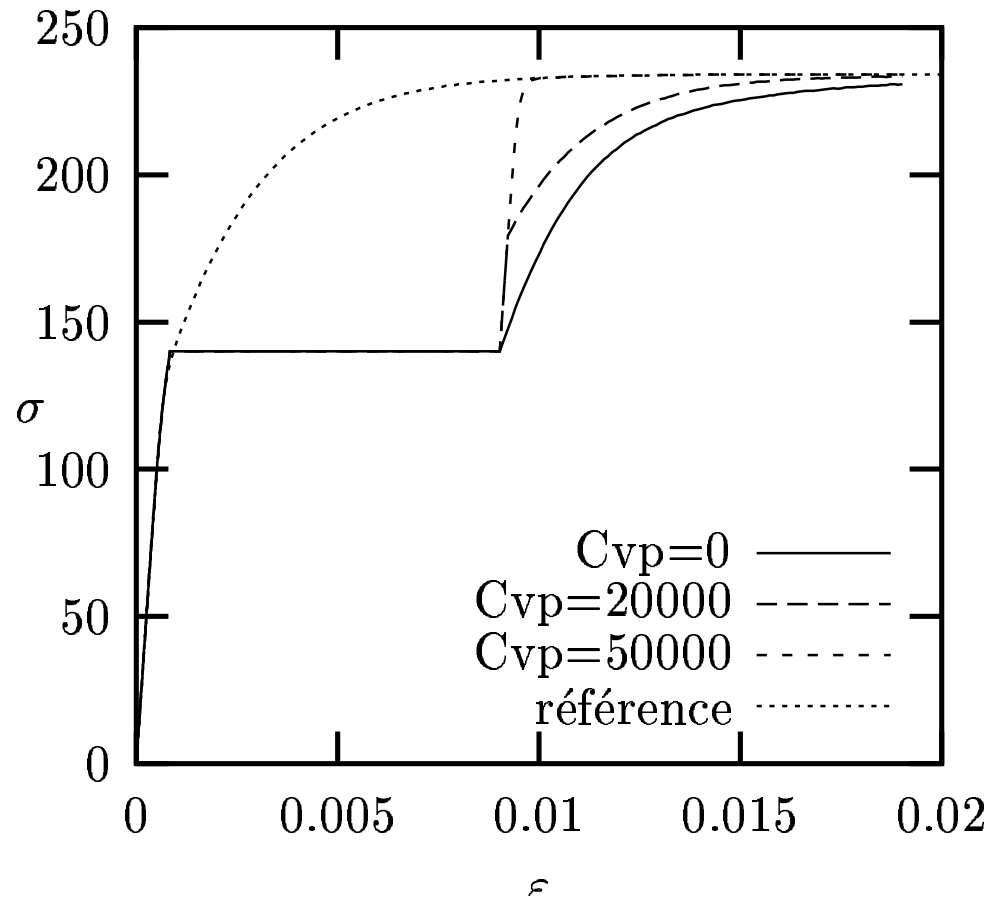
Tensile curves at various strain rates



Amount of plasticity in inelastic strain

$$K = 500; n = 7; R_0^v = 80; C_v = 10000; D = 100; R_0^p = 140; C_p = 20000; D = 200$$

2M2C-VP model: Influence of the coupling term



(units : MPa, s)

viscosity :

$K = 500 ; n = 7$

isotropic viscous :

$R_0 = 0$

kinematic viscous :

$C = 50000 ; D = 500$

isotropic plastic :

$R_0 = 140$

kinematic plastic :

$C = 50000 ; D = 500$

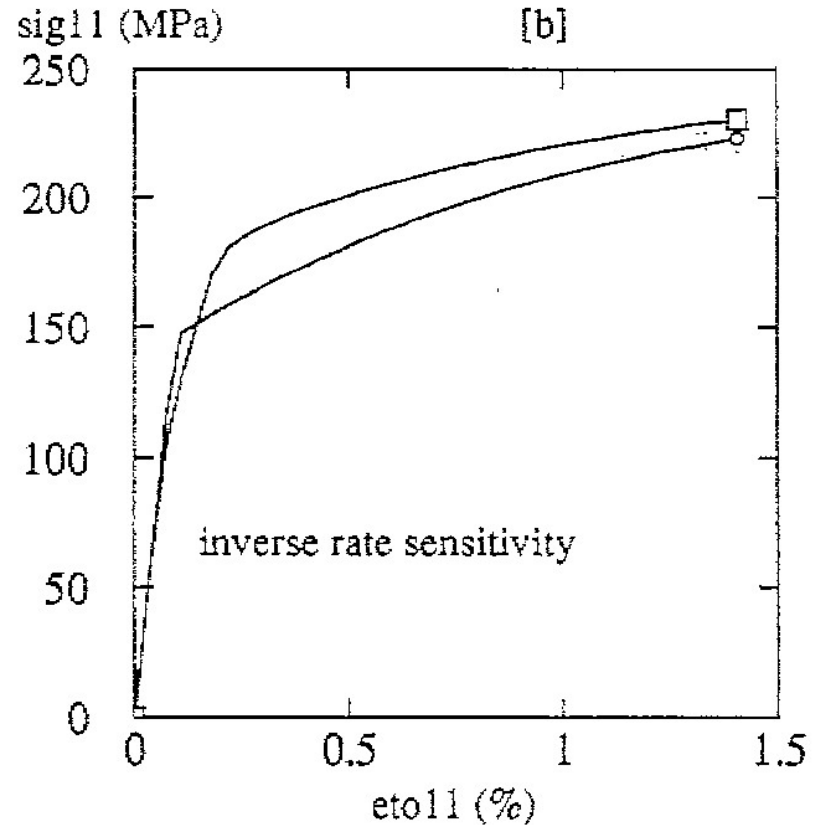
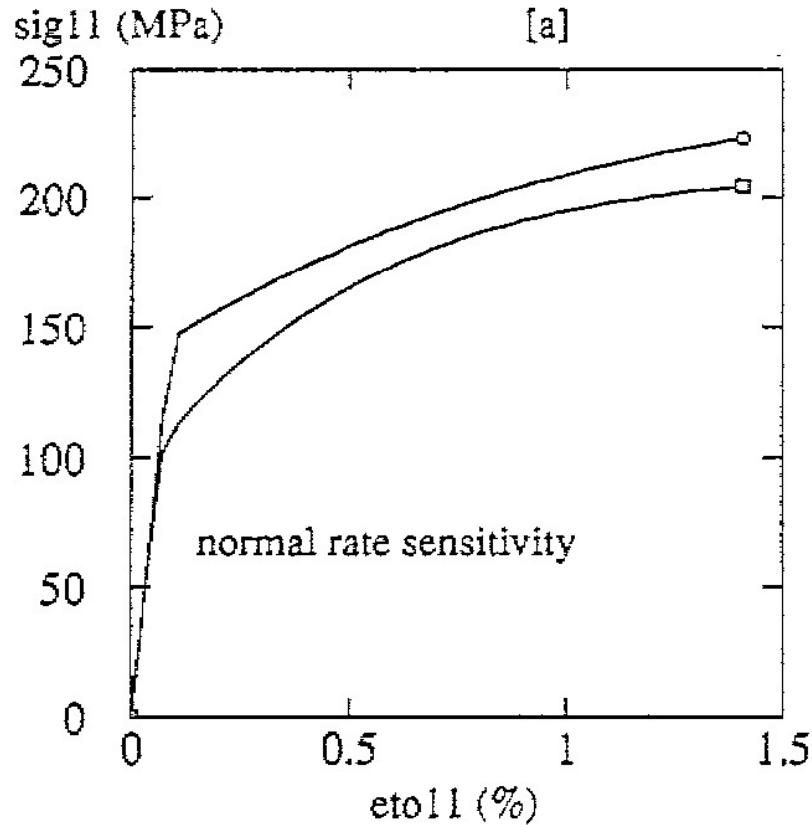
Creep 555 h at 140 MPa, then tension at $\dot{\epsilon} = 10^{-4} s^{-1}$

reference in tension at $\dot{\epsilon} = 10^{-4} s^{-1}$

2M2C-VP model: Inverse strain rate effect (1)

○ $\dot{\epsilon} = 10^{-3} s^{-1}$

□ $\dot{\epsilon} = 10^{-6} s^{-1}$



Normal rate sensitivity if $C_p < C_v < C_{vp}$

$$C_p = 10000 < C_v = 20000 < C_{vp} = 40000$$

$$D_p = 100, D_v = 200$$

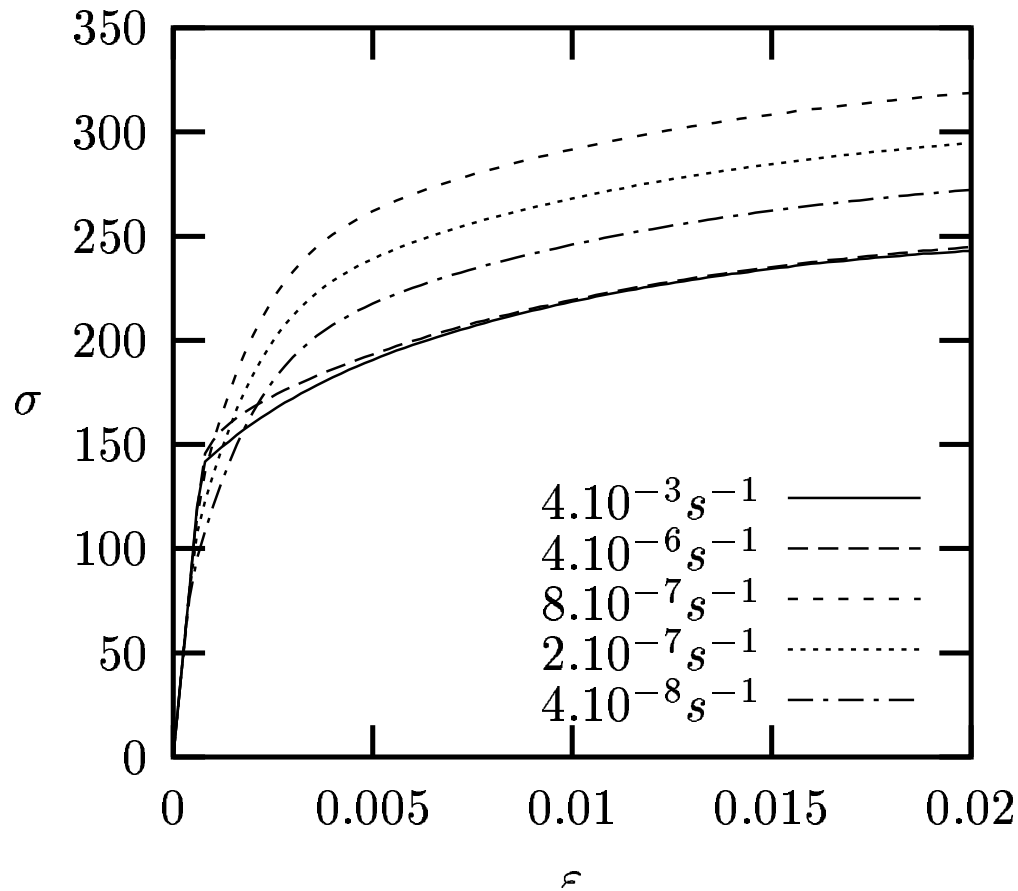
Other coefficients: $K = 700, n = 7.2; R_0^v = 0; R_0^p = 140$

Inverse rate sensitivity if $C_p < C_{vp} \ll C_v$

$$C_p = 10000 < C_{vp} = 40000 < C_v = 100000$$

$$D_p = 400, D_v = 100$$

2M2C-VP model: Inverse strain rate effect (1)



$$K = 1000, n = 7$$

$$R_0^v = 0$$

$$C_{1v} = 10000, D_{1v} = 100$$

$$C_{2v} = 100000, D_{2v} = 1000$$

$$R_0^p = 140$$

$$C_{1p} = 10000, D_{1p} = 100$$

$$C_{2p} = 10000, D_{2p} = 50$$

$$C_{1vp} = 20000$$

$$C_{2vp} = 100000$$

2M1C model: state variables and flow

Free energy, *idem* 2M2C:

$$\rho\psi = \frac{1}{3} \sum_I \sum_J C_{IJ} \underline{\alpha}^I : \underline{\alpha}^J$$

$$+ \frac{1}{2} \sum_I b_I Q_I (r^I)^2$$

$$\underline{\mathbf{X}}^I = \frac{2}{3} \sum_J C_{IJ} \underline{\alpha}^J$$

$$R^I = b_I Q_I r^I$$

Flow:

$$\Omega \equiv \Omega(f)$$

$$f = (J(\underline{\sigma} - \underline{\mathbf{X}}^1)^2 + J(\underline{\sigma} - \underline{\mathbf{X}}^2)^2)^{1/2} - R - R_0$$

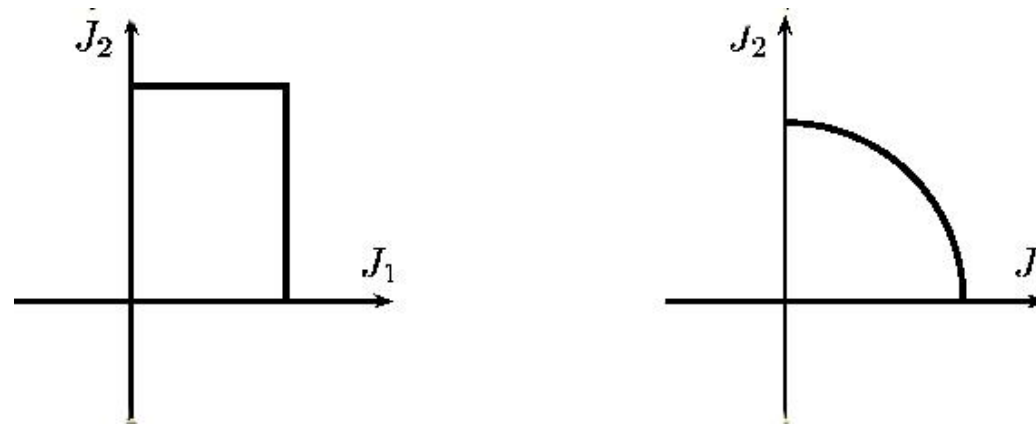
$$\underline{\dot{\epsilon}}^p = \frac{\partial \Omega}{\partial f} \underline{n}$$

$$\text{with } \underline{n} = \frac{J_1 \underline{n}^1 + J_2 \underline{n}^2}{(J_1^2 + J_2^2)^{1/2}}$$

Each flow can be viscoplastic or plastic

2M1C model: features

- Comparison between 2M2C (left) and 2M1C (right)



- Viscoplastic or plastic formulation
- Interesting for the properties under *ratchetting* loadings

2M1C-P: plastic multiplier

$$\dot{\lambda} = \left\langle \frac{(J_1 \underline{\mathbf{n}}^1 + J_2 \underline{\mathbf{n}}^2) : \dot{\underline{\boldsymbol{\sigma}}}}{h_R + h_{X1} + h_{X2}} \right\rangle$$

with :

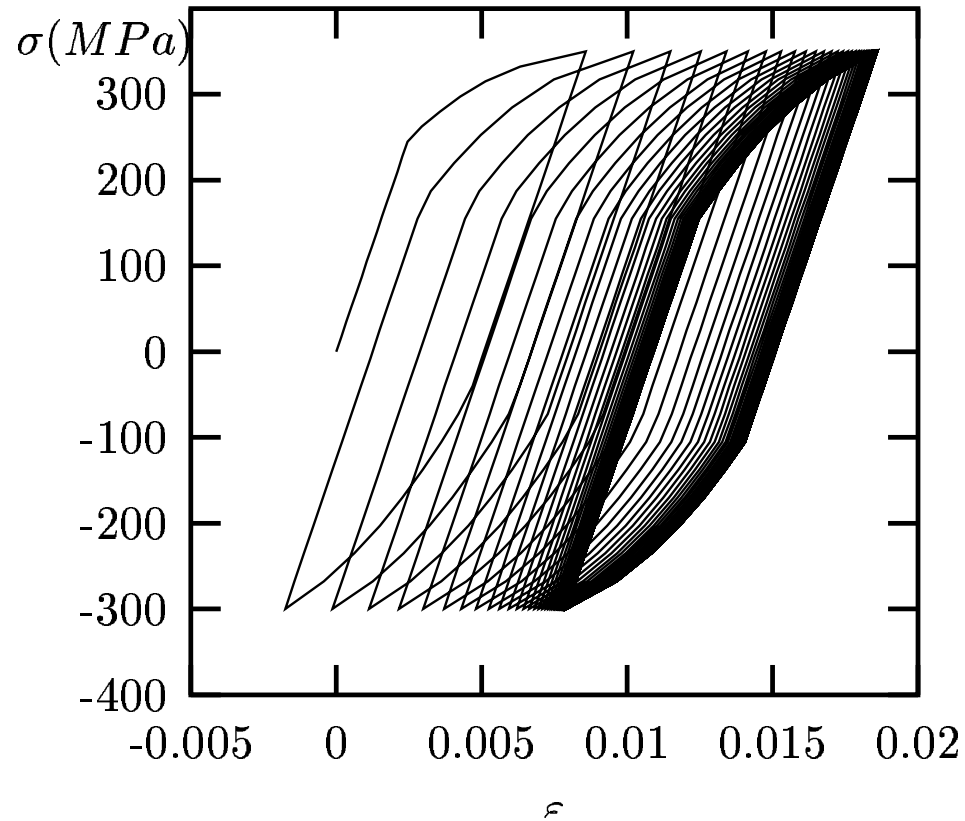
$$h_R = b(Q - R) R$$

$$h_{X1} = \frac{2}{3} \left(\underline{\mathbf{n}}^1 - \frac{3D_1}{2C_{11}} \underline{\mathbf{X}}^1 \right) : (C_{11} J_1 \underline{\mathbf{n}}^1 + C_{12} J_2 \underline{\mathbf{n}}^2)$$

$$h_{X2} = \frac{2}{3} \left(\underline{\mathbf{n}}^2 - \frac{3D_2}{2C_{22}} \underline{\mathbf{X}}^2 \right) : (C_{12} J_1 \underline{\mathbf{n}}^1 + C_{22} J_2 \underline{\mathbf{n}}^2)$$

No ratchetting, except if $C_{11}C_{22} - C_{12}^2 = 0$

2M1C-P: Plastic shakedown



coefficients (MPa,s)

viscosité :

$$n=2, K=5$$

cinématique I :

$$C_{11} = 2000 ; D_1 = 0$$

cinématique II :

$$C_{22} = 200000 ; D_2 = 0$$

isotrope :

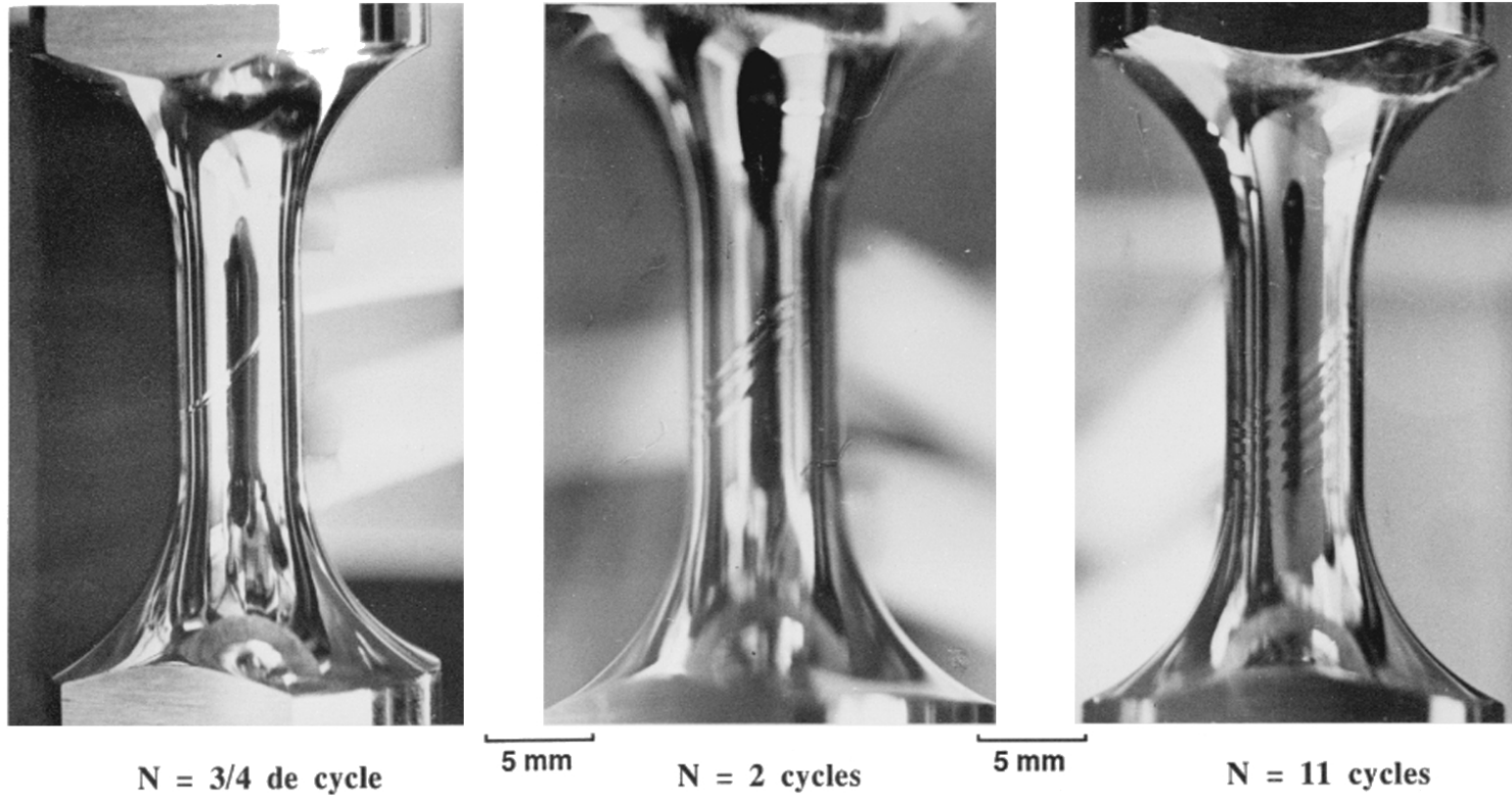
$$R_0 = 350$$

couplage :

$$C_{12} = -20000$$

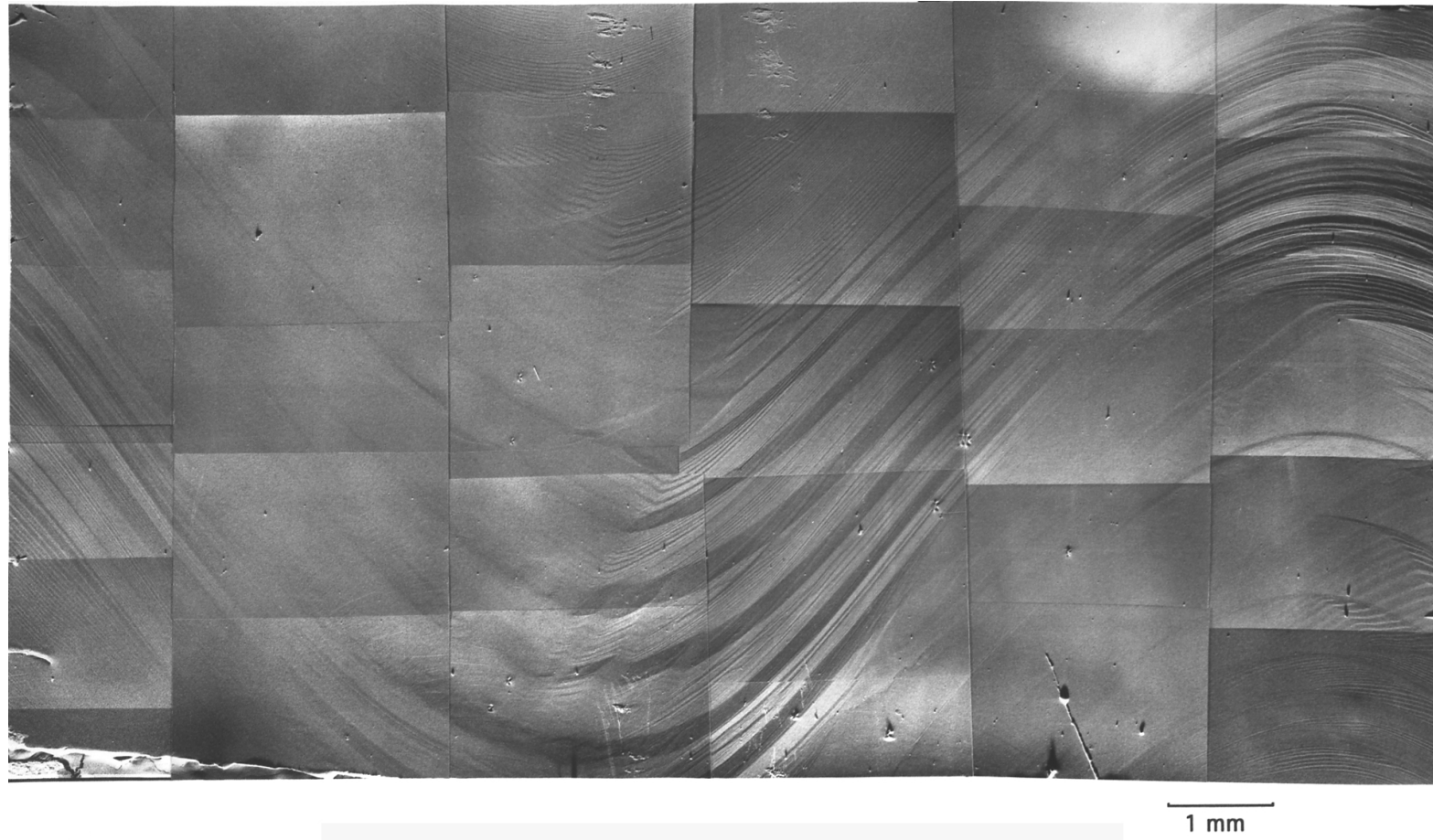
Steady state presenting an open loop under non symmetrical loading

Single crystal specimens



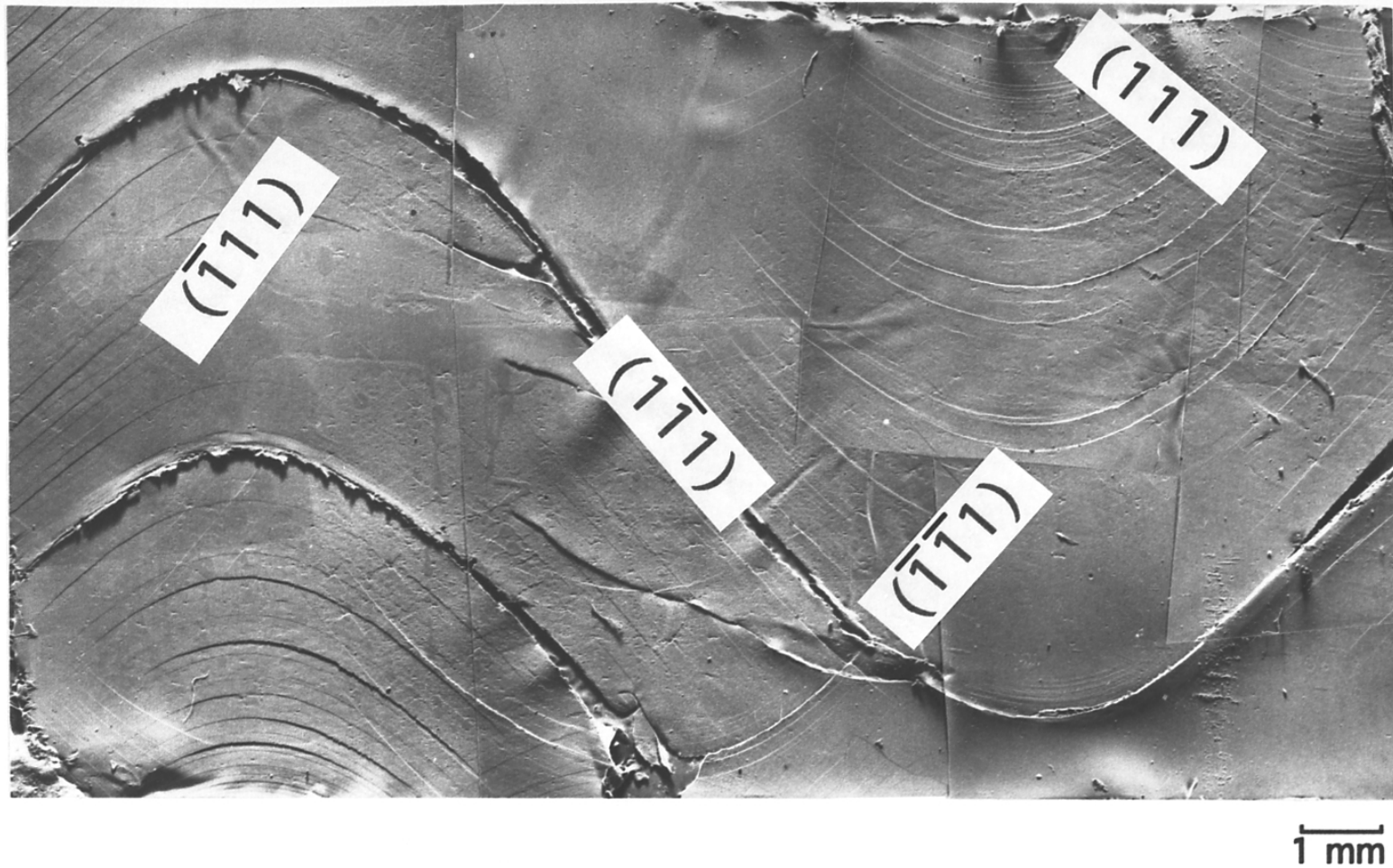
A reduced number of mechanisms, the slip systems (PhD F.Hanriot, 1993)

Replica of a tensile single crystal specimens



Initial yield (PhD F.Hanriot, 1993)

Replica of a tensile single crystal specimens (2)



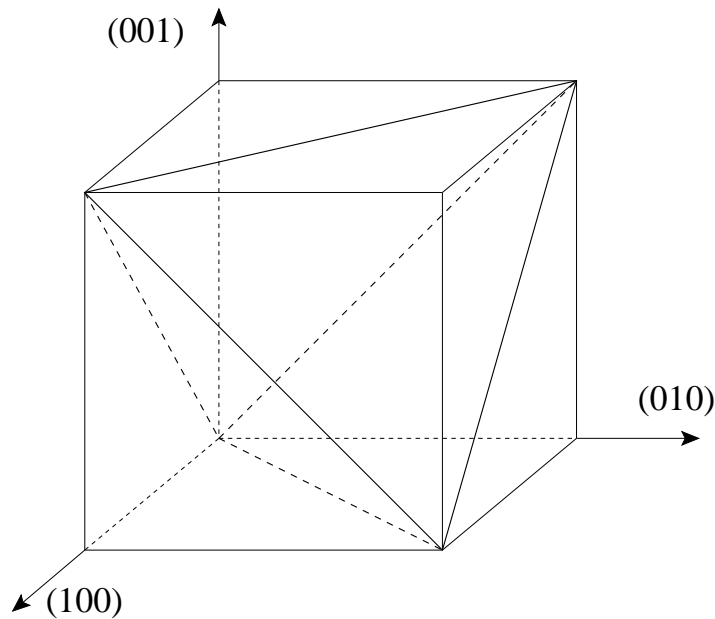
End of life (PhD F.Hanriot, 1993)

Slip systems, Schmid law

Back to illustrations A slip system s is characterized by its plane (vector \underline{n}) and its slip direction (vector \underline{m}). The resolved shear stress τ^s is expressed as:

$$\tau^s = \sigma_{ij} n_i m_j = \frac{1}{2} \sigma_{ij} (n_i m_j + m_i n_j) = \sigma_{ij} m_{ij}$$

Let us define the *orientation tensor* by $\underline{m} = \frac{1}{2} (\underline{n} \otimes \underline{m} + \underline{m} \otimes \underline{n})$



The four octahedral planes in a cubic crystal

The *Schmid law* assumes that slip occurs for a system when the resolved shear stress reaches a given threshold, the critical resolved shear stress, denoted here by τ_c . The plasticity criterion is then the result of a collection of criteria, the expression of which is linear in stress:

$$|\tau^s| - \tau_c = 0 \quad \text{ou encore} \quad \underline{\sigma} : \underline{m}^s - \tau_c = 0$$

Definition of the slip systems in a FCC single crystal

The four octahedral planes of a cubic crystal previously shown have three systems. Here is the collection of the 12 systems, defined by \underline{n} and \underline{m} :

num syst	1	2	3	4	5	6	7	8	9	10	11	12	
$\sqrt{3}n_1$	1	1	1	1	1	1	-1	-1	-1	1	1	1	
$\sqrt{3}n_2$	1	1	1	-1	-1	-1	1	1	1	1	1	1	
$\sqrt{3}n_3$	1	1	1	$\sqrt{3}$	1	1	1	1	1	1	-1	-1	-1
$\sqrt{2}m_1$	-1	0	-1	-1	0	1	0	1	1	-1	1	0	
$\sqrt{2}m_2$	0	-1	1	0	1	1	-1	1	0	1	0	1	
$\sqrt{2}m_3$	1	1	0	$\sqrt{2}$	1	1	0	1	0	1	0	1	

Orientation tensors of a FCC single crystal

num syst	1	2	3	4	5	6	7	8	9	10	11	12
$\sqrt{6}m_{11}$	-1	0	-1	-1	0	1	0	-1	-1	-1	1	0
$\sqrt{6}m_{22}$	0	-1	1	0	-1	-1	-1	1	0	1	0	1
$\sqrt{6}m_{33}$	1	1	0	1	1	0	1	0	1	0	-1	-1
$2\sqrt{3}m_{12}$	-1	-1	0	1	1	0	1	0	1	0	1	1
$2\sqrt{3}m_{23}$	1	0	1	-1	0	1	0	1	1	-1	1	0
$2\sqrt{3}m_{31}$	0	1	-1	0	1	1	-1	1	0	1	0	1

- If the only non zero terms of the stress tensor are σ_{11} , σ_{12} et σ_{21} , the criterion writes:

$$|\sigma_{11}m_{11} + 2\sigma_{12}m_{12}| - \tau_c = 0$$

- If the only non zero terms of the stress tensor are σ_{11} , et σ_{33} , the criterion writes:

$$|\sigma_{11}m_{11} + \sigma_{33}m_{33}| - \tau_c = 0$$

Resolved shear stress for $\sigma_{11}-\sigma_{12}$ and $\sigma_{11}-\sigma_{33}$ in a FCC single crystal

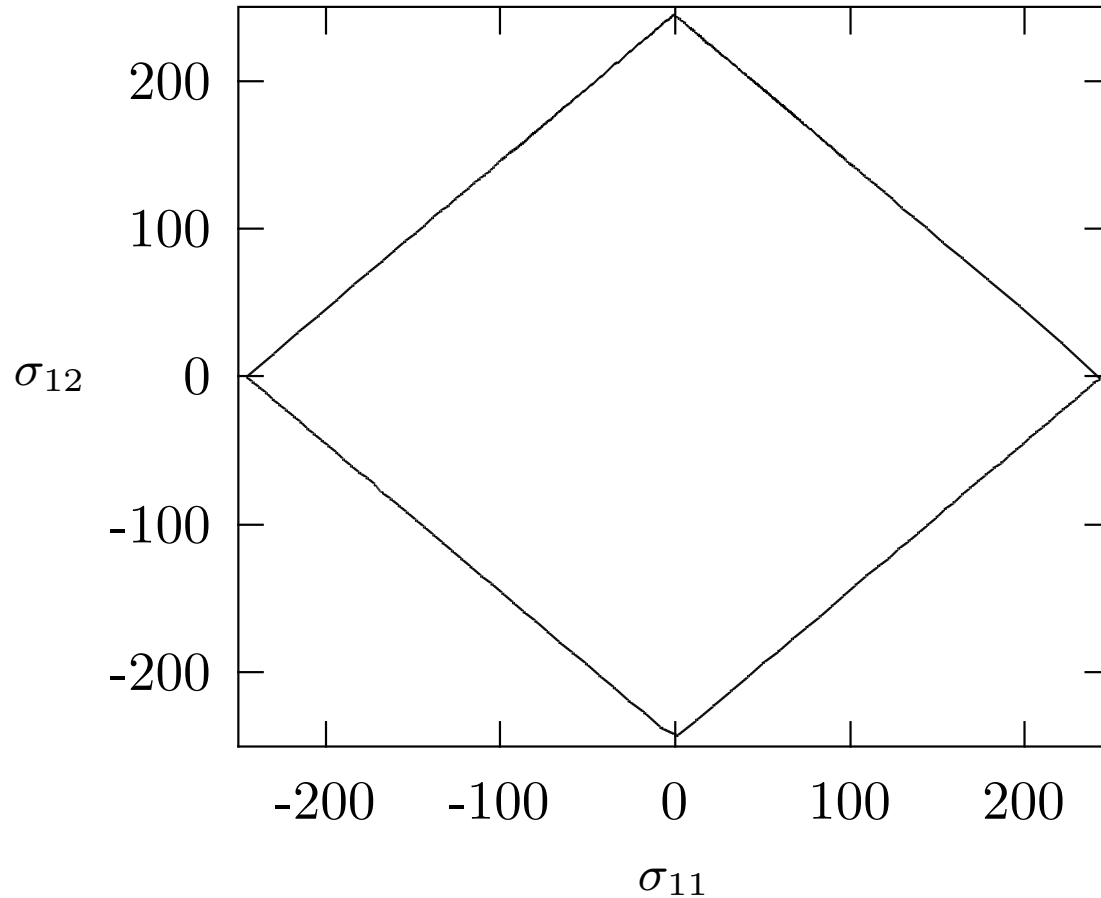
For the σ_{11} et σ_{12} stresses, the τ^s values are respectively:

num syst	1	2	3	4	5	6
τ^s	$-\sigma_{11} - \sigma_{12}$	$-\sigma_{12}$	$-\sigma_{11}$	$-\sigma_{11} + \sigma_{12}$	σ_{12}	σ_{11}
num syst	7	8	9	10	11	12
τ^s	σ_{12}	$-\sigma_{11}$	$-\sigma_{11} + \sigma_{12}$	$-\sigma_{11}$	$\sigma_{11} + \sigma_{12}$	σ_{12}

And for σ_{11} et σ_{33} stresses,

num syst	1	2	3	4	5	6
τ^s	$-\sigma_{11} + \sigma_{33}$	σ_{33}	$-\sigma_{11}$	$-\sigma_{11} + \sigma_{33}$	σ_{33}	σ_{11}
num syst	7	8	9	10	11	12
τ^s	σ_{33}	$-\sigma_{11}$	$-\sigma_{11} + \sigma_{33}$	$-\sigma_{11}$	$\sigma_{11} - \sigma_{33}$	$-\sigma_{33}$

Elastic domain σ_{11} – σ_{12} of a FCC single crystal



For tension–shear loading, the domain is then defined by 4 systems:

- systems 1 and 11 give :

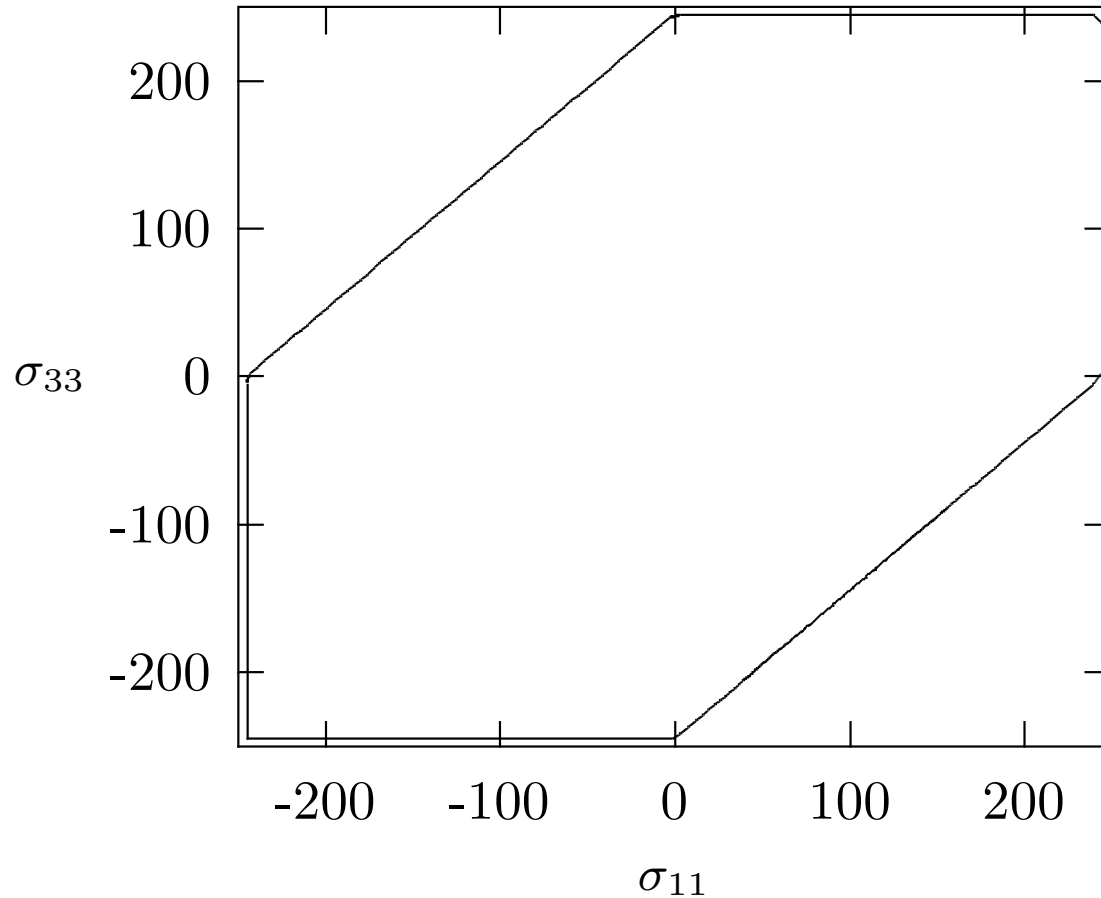
$$|\sigma_{11} + \sigma_{12}| = \tau_c \sqrt{6}$$

- systems 4 and 9 give :

$$|\sigma_{11} - \sigma_{12}| = \tau_c \sqrt{6}$$

This figure is computed for $\tau_c = 100$ MPa.

Elastic domain $\sigma_{11}-\sigma_{33}$ of a FCC single crystal



For biaxial tension:

- systems 1, 4, 9 et 11 :

$$|\sigma_{11} - \sigma_{33}| = \tau_c \sqrt{6}$$

- systems 3, 6, 8, 10 :

$$|\sigma_{11}| = \tau_c \sqrt{6}$$

- systems 2, 5, 7, 13 :

$$|\sigma_{33}| = \tau_c \sqrt{6}$$

This figure is computed for $\tau_c = 100$ MPa.

General formulation

- State variables; α^s and ρ^s in the free energy

$$\rho\psi = \frac{1}{2} c \sum_s (\alpha^s)^2 + \frac{1}{2} Q \sum_r \sum_s h_{rs} \rho^r \rho^s$$

- Hardening variables x^s and r^s defined as partial derivatives:

$$x^r = c\alpha^r \quad ; \quad r^r = bQ \sum_s h_{rs} \rho^s$$

- Criterion

$$f^r = |\tau^r - x^r| - r^r - \tau_0$$

$$\text{with } \tau^r = \underline{\underline{\sigma}} : \underline{\underline{m}}^r = \underline{\underline{\sigma}} : \frac{1}{2} (\underline{\underline{l}}^r \otimes \underline{\underline{n}}^r + \underline{\underline{n}}^r \otimes \underline{\underline{l}}^r)$$

Viscoplastic formulation

- Viscoplastic potential

$$\Omega = \sum_r \Omega_r(f^r) = \frac{K}{n+1} \sum_r \left\langle \frac{f^r}{K} \right\rangle^{n+1}$$

- Viscoplastic flow

$$\tilde{\dot{\boldsymbol{\epsilon}}}^p = \frac{\partial \Omega}{\partial \tilde{\boldsymbol{\sigma}}} = \sum_r \dot{\gamma}^r : \tilde{\boldsymbol{m}}^r$$

$$\text{avec } \dot{v}^r = \frac{\partial \Omega}{\partial f^r} = \left\langle \frac{f^r}{K} \right\rangle^n$$

$$\text{et } \dot{\gamma}^r = \dot{v}^r \text{signe}(\tau^r - x^r)$$

- Hardening (non associated model)

$$\dot{\alpha}^r = (\text{signe}(\tau^r - x^r) - d\alpha^r)\dot{v}^r$$

$$\dot{\rho}^r = (1 - b\rho^r)\dot{v}^r$$

Operational form of the single crystal model

$$\dot{\underline{\xi}} = \dot{\underline{\xi}}^e + \dot{\underline{\xi}}^p$$

$$\tau^s = \underline{\sigma}^g : \underline{\mathbf{m}}^s = \frac{1}{2} \underline{\sigma}^g : (\underline{\mathbf{n}}^s \otimes \underline{\mathbf{l}}^s + \underline{\mathbf{l}}^s \otimes \underline{\mathbf{n}}^s)$$

$$x^s = c \alpha^s \quad ; \quad r^s = R_0 + Q \sum_r h_{rs} \{1 - e^{-bv^r}\}$$

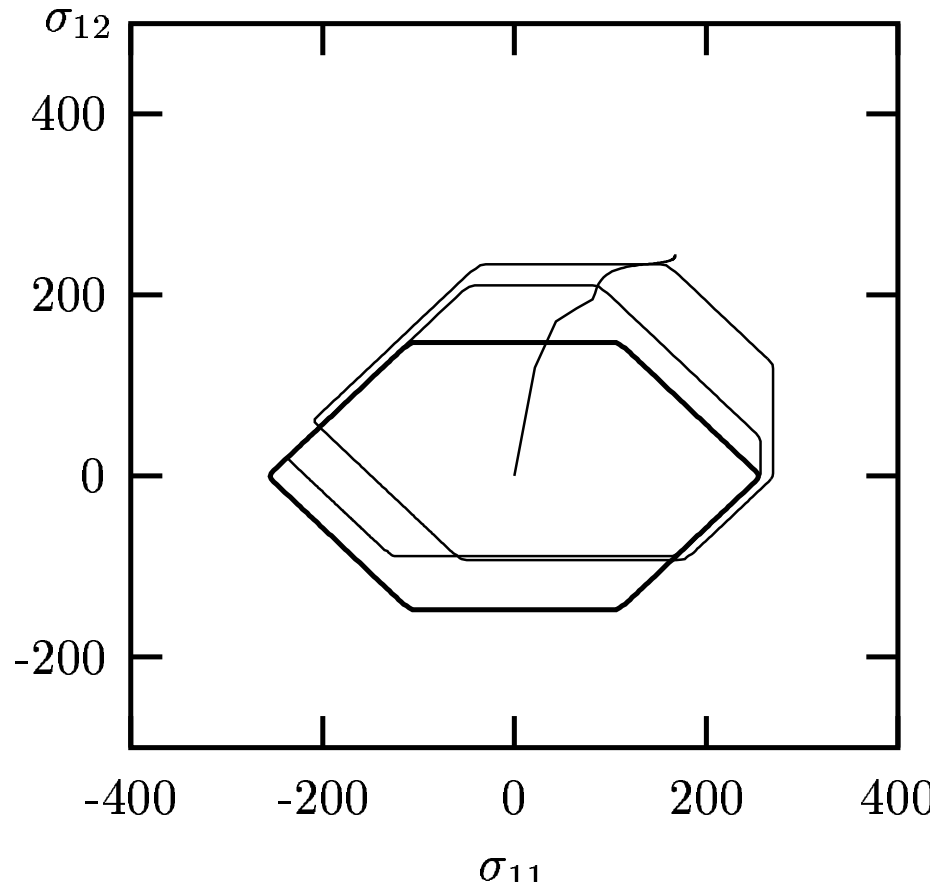
$$\dot{\gamma}^s = \dot{v}^s \text{sign}(\tau^s - x^s) \quad ; \quad \dot{\underline{\xi}}^p = \sum_s \underline{\mathbf{m}}^s \dot{\gamma}^s$$

$$\dot{v}^s = \left\langle \frac{|\tau^s - x^s| - r^s}{K} \right\rangle^n \quad \text{with } \langle x \rangle = \text{Max}(x, 0) \quad \text{and} \quad v^s(t=0) = 0$$

$$\dot{\alpha}^s = \dot{\gamma}^s - d \alpha^s \dot{v}^s \quad \text{with} \quad \alpha^s(t=0) = 0$$

Subsequent yield surfaces for a prescribed strain path

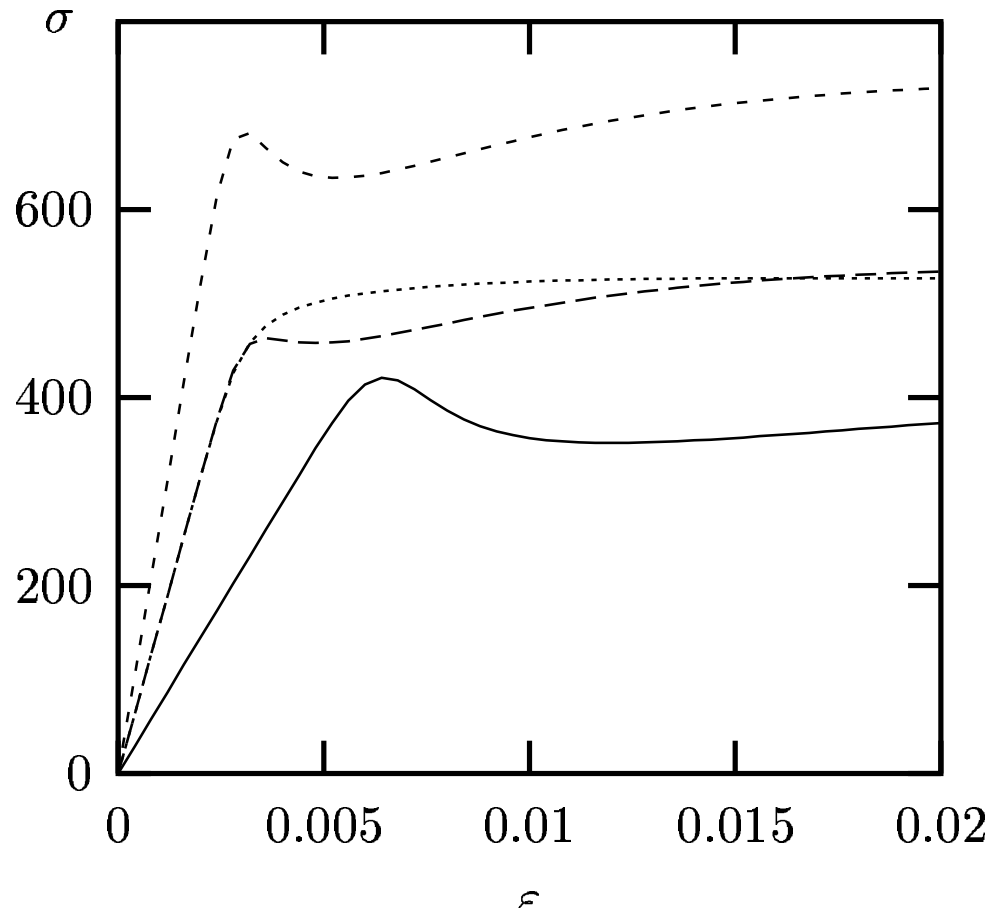
Prescribed strain such as $\varepsilon_{12}^{max} = 2\varepsilon_{11}^{max}$



coeff (MPa,s)	octa	cube
τ_0	100	100
Q	20	10
b	10	10
c	10000	35000
d	200	700
K	20	20
n	2	2
h_{ij}	1	1

Two slip system families: octahedral, cubic

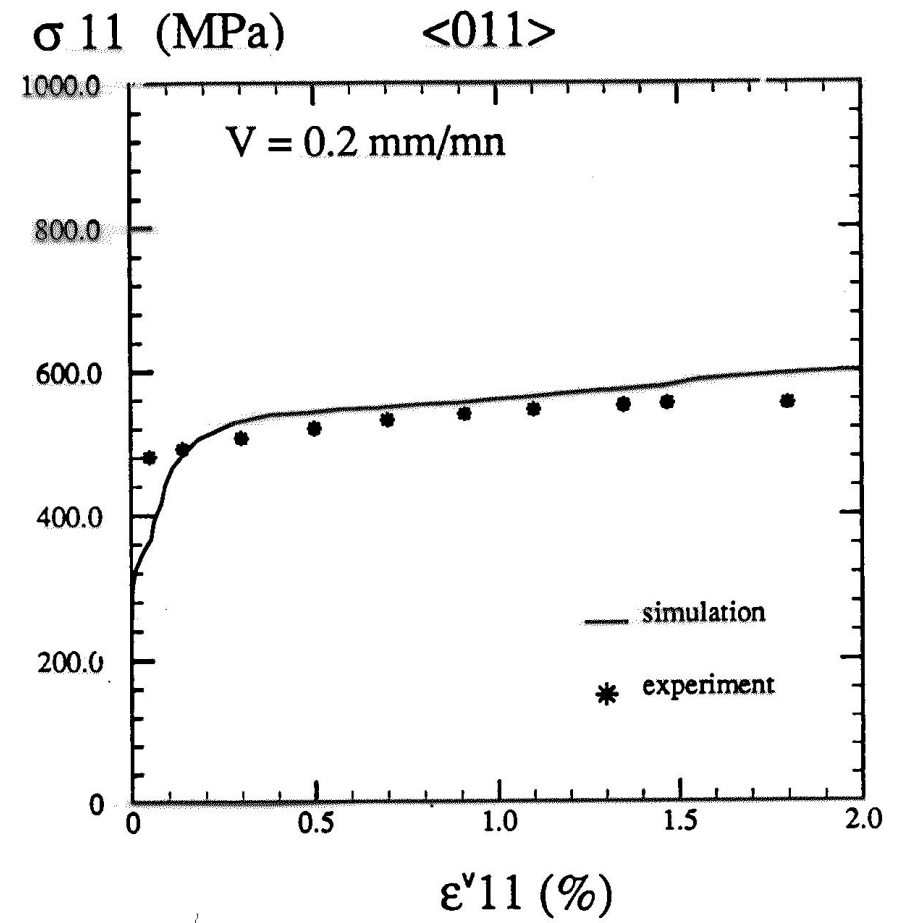
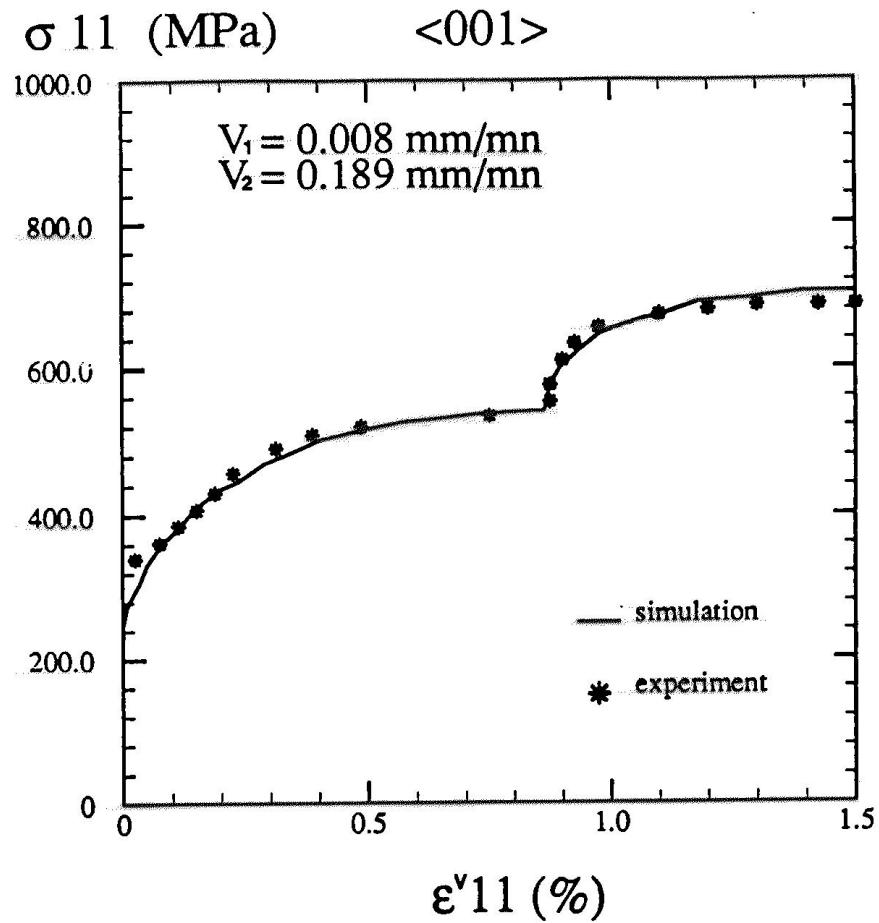
Tensile curves for various crystallographic directions



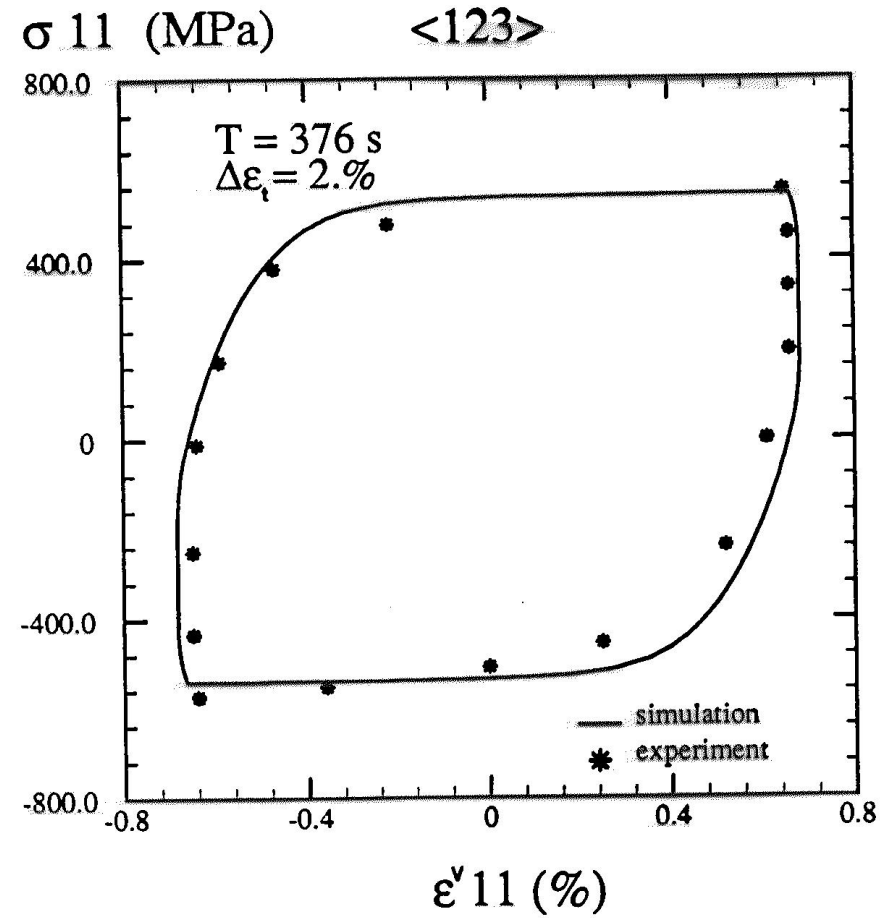
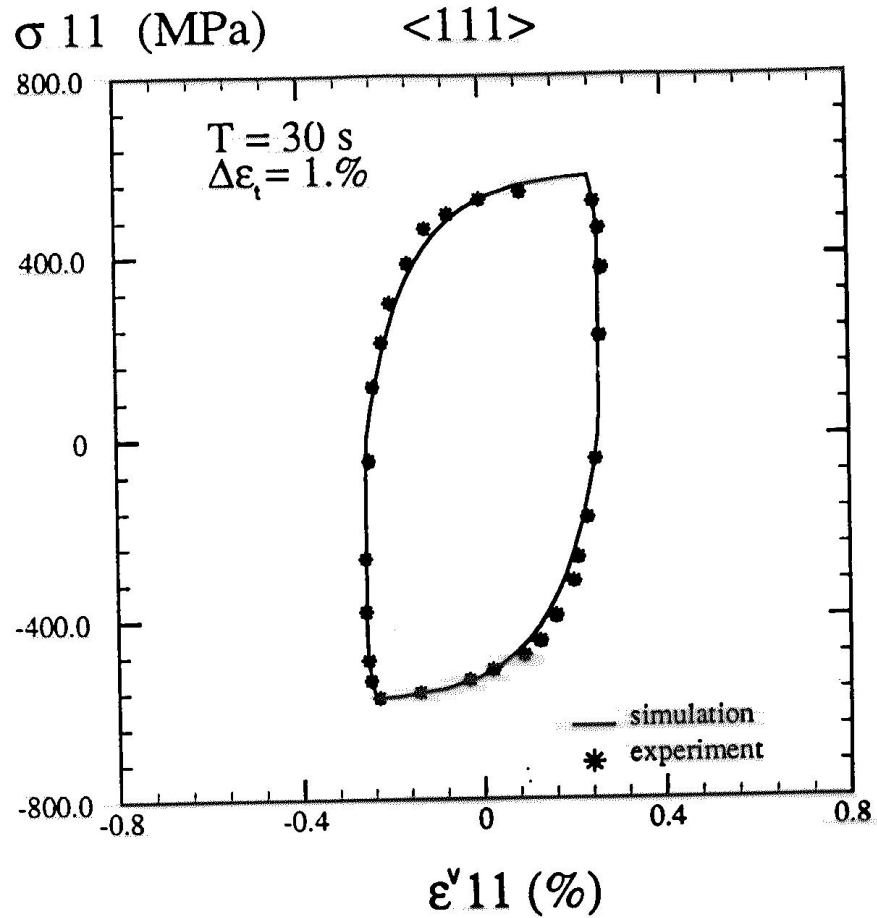
	coeff (MPa,s)	syst. octa
001	τ_0	100
011	Q	-10
111	b	1000
123	c	20000
	d	300
	K	500
	n	5
	h_{ij}	1

Octahedral slip systems only

Monotonic tests on AM1 superalloy



Cyclic tests on AM1 superalloy



Equivalence between single crystal and von Mises

- Single crystal model in multiple slip, with N equivalent slip systems, Schmid factor m

$$\dot{\tilde{\epsilon}}^P = \sum_s \tilde{m}^s \dot{\gamma}^s = \sum_s \tilde{m}^s \left\langle \frac{|\tau^s - x^s| - r^s}{k} \right\rangle^n$$

becomes

$$\dot{\epsilon}^P = Mm\dot{\gamma}^s = Mm \left\langle \frac{m(\sigma - x) - r}{k} \right\rangle^n$$

- Equivalent to a macroscopic model

$$\dot{\epsilon}^P = \left\langle \frac{(\sigma - X) - R}{K} \right\rangle^n \quad \text{with } K = \frac{k}{m} \frac{1}{mM}^{1/n}, \quad X = \frac{x}{m}, \quad R = \frac{r}{m}$$

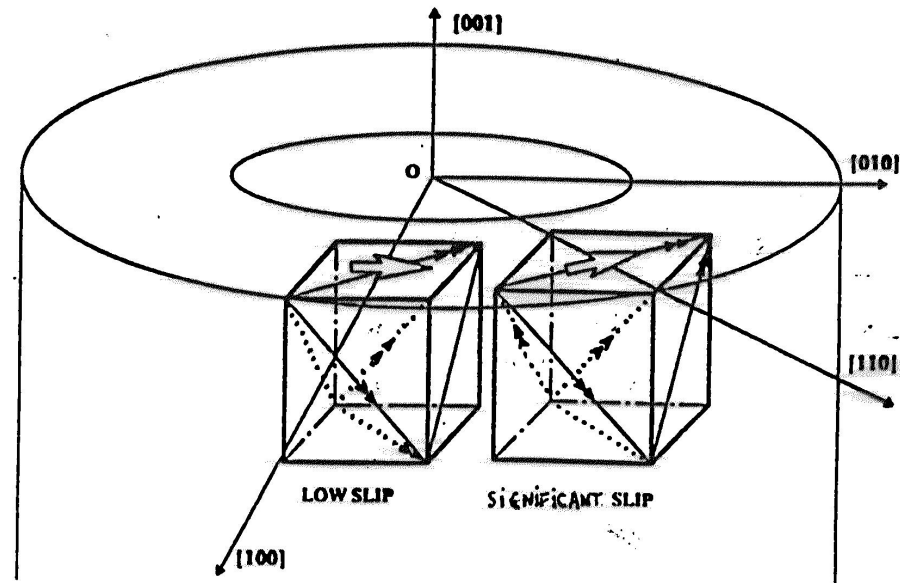
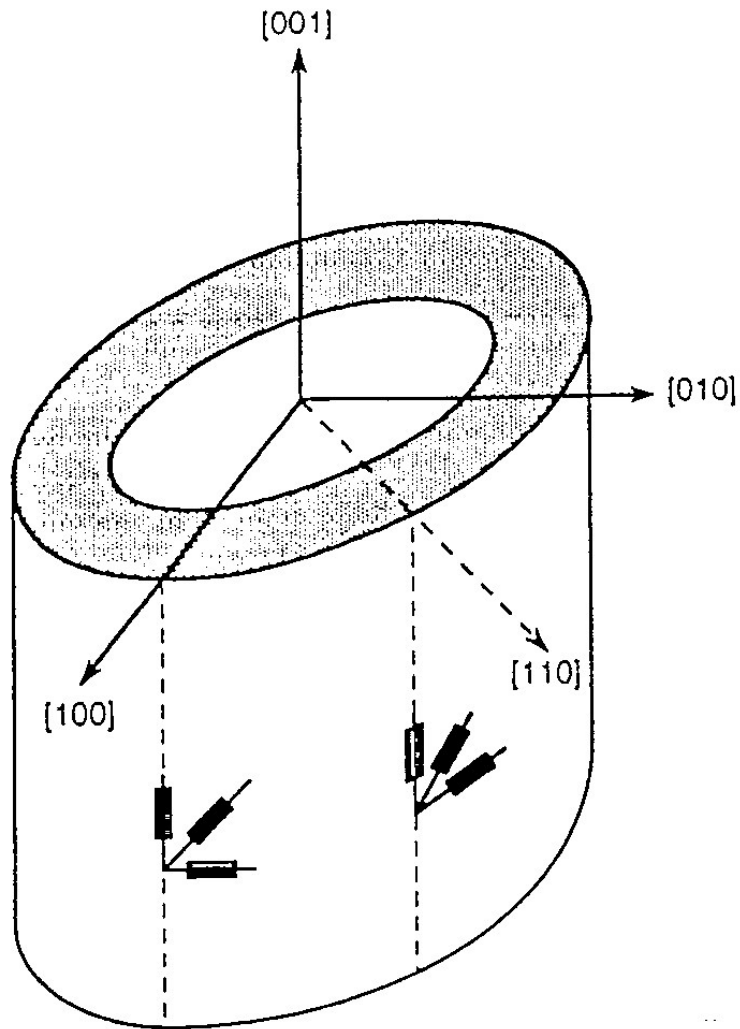
Equivalence between single crystal and von Mises (2)

Coefficient	Value for multiple slip (m,M)	Value for 001 tension $N = 8, m = 1/\sqrt{6}$	Value for 111 tension $N = 6, m = \sqrt{2}/3$
K	$\frac{k}{m(Mm)^{1/n}}$	$\frac{\sqrt{6}k}{(8/\sqrt{6})^{1/n}}$	$\frac{3k}{2^{(n+1)/2n}}$
R_0	$\frac{r_o}{m}$	$\sqrt{6}r_o$	$\frac{3r_o}{\sqrt{2}}$
Q	$\frac{Q}{m}$	$\sqrt{6}Q$	$\frac{3Q}{\sqrt{2}}$
b	$\frac{b}{mM}$	$\frac{\sqrt{6}b}{8}$	$\frac{b}{\sqrt{2}}$
C	$\frac{c}{Mm^2}$	$\frac{3c}{4}$	$\frac{3c}{2}$
D	$\frac{d}{Mm}$	$\frac{\sqrt{6}d}{8}$	$\frac{d}{\sqrt{2}}$

There is a relation between the coefficients of a macro model and a crystal plasticity model

Single crystal tube in torsion

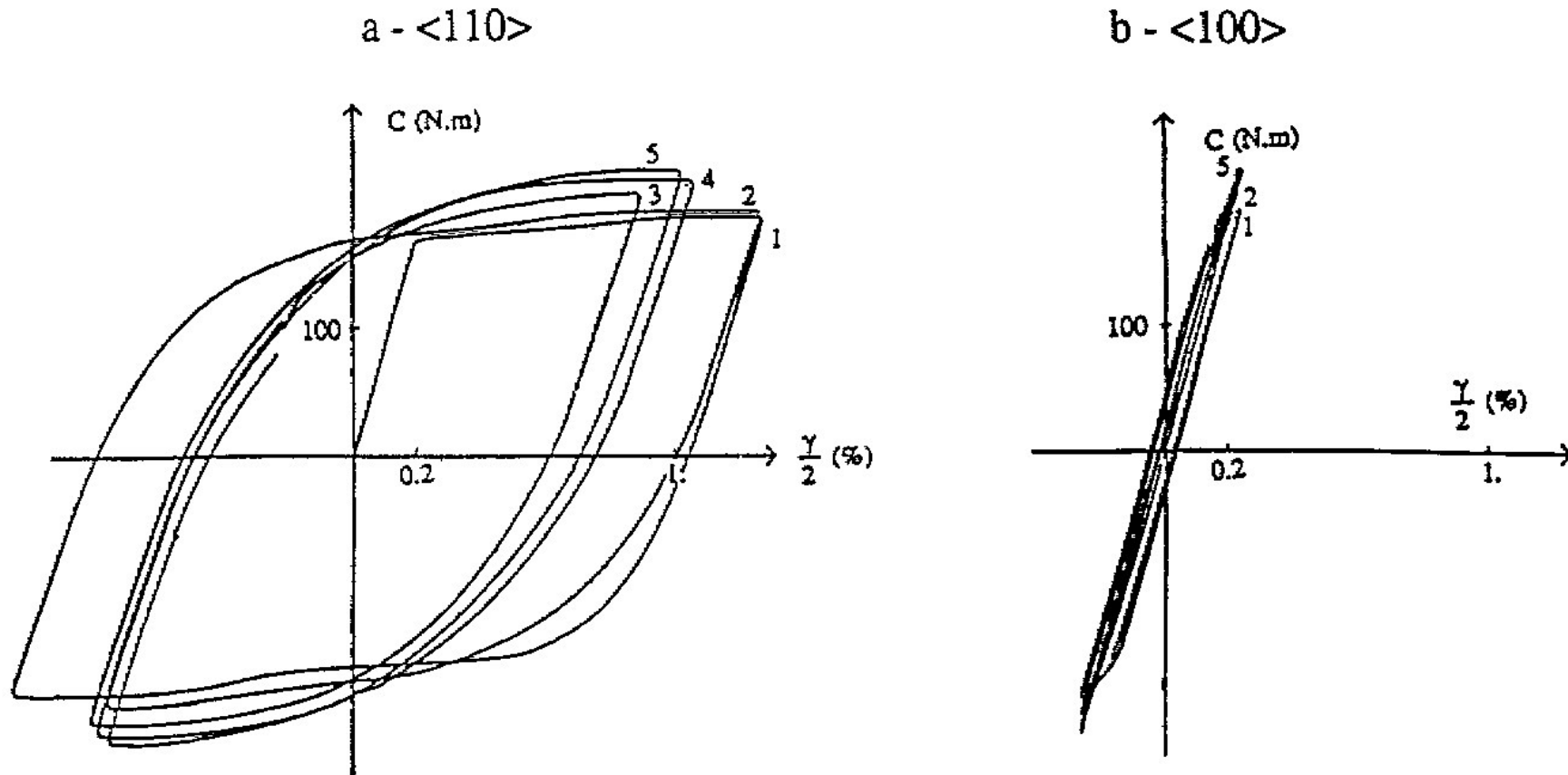
001 cristallographic axis is in the direction of the tube axis



100 is a hard zone, 110 is a soft area

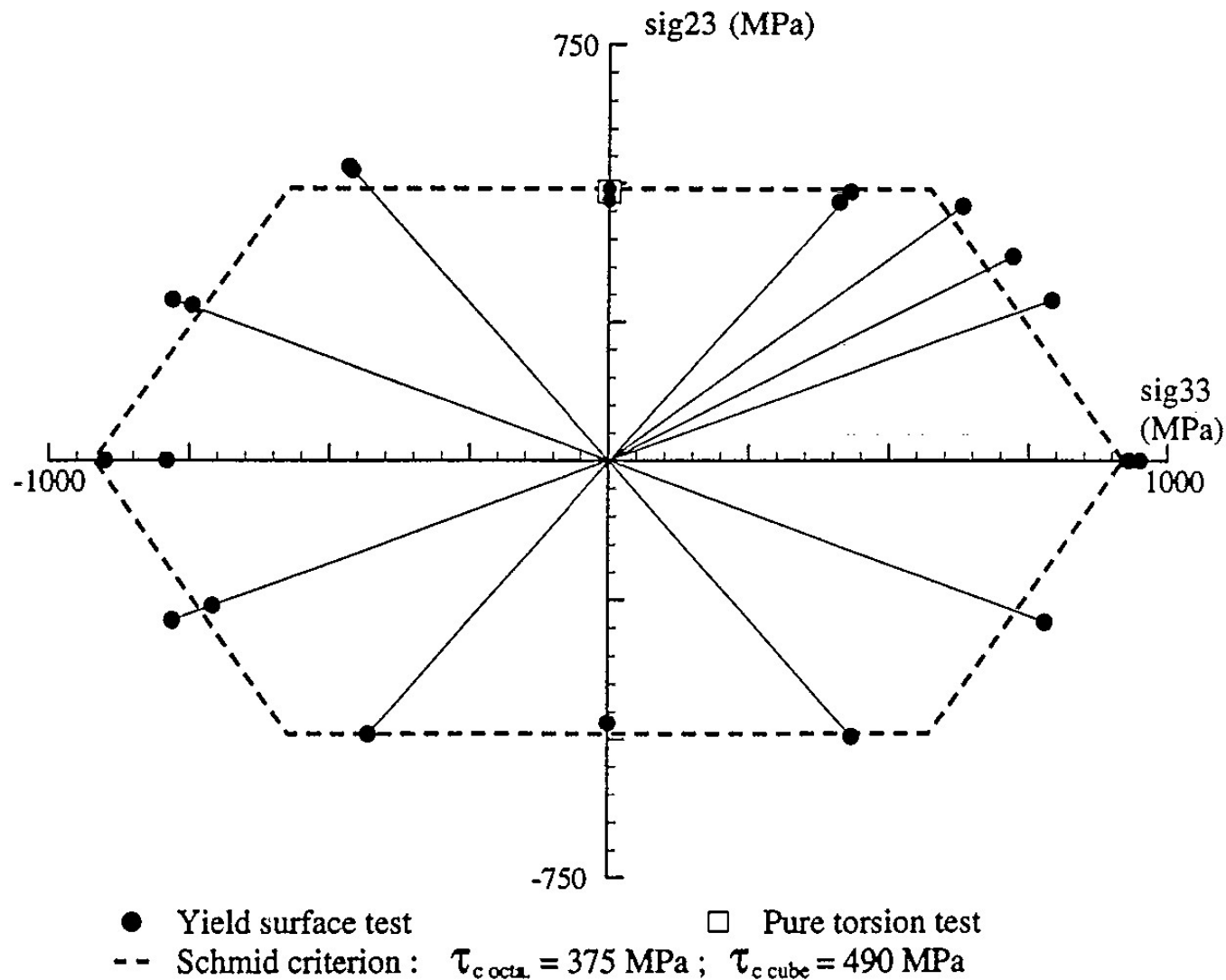
Strain jauges are in 100 and 001 areas

Single crystal tube in torsion (2)



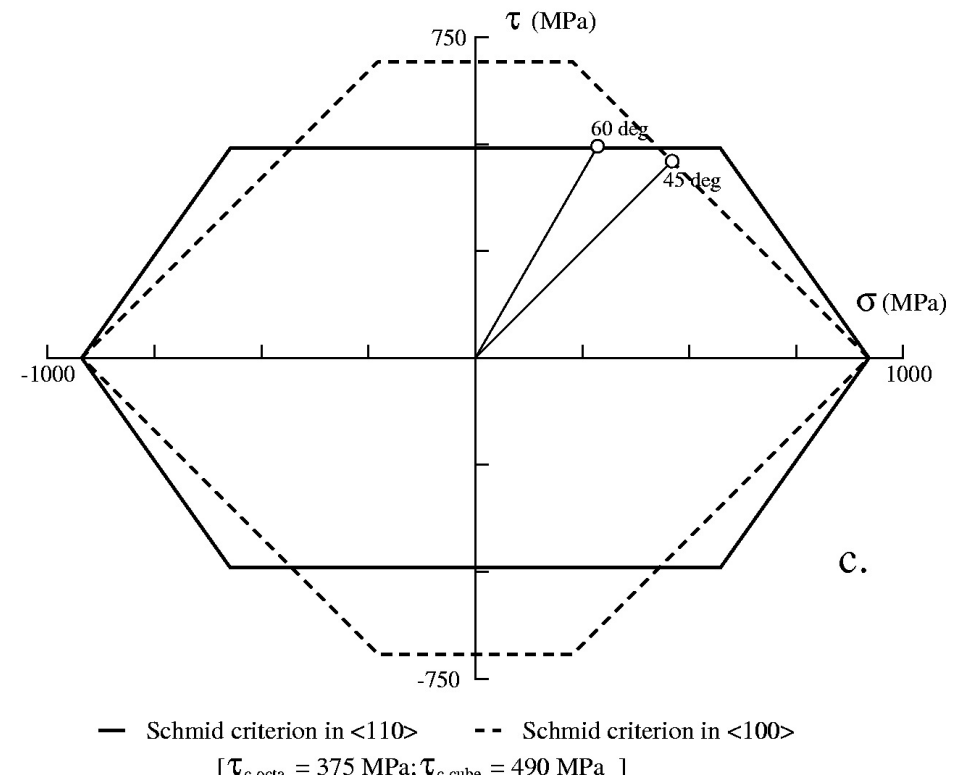
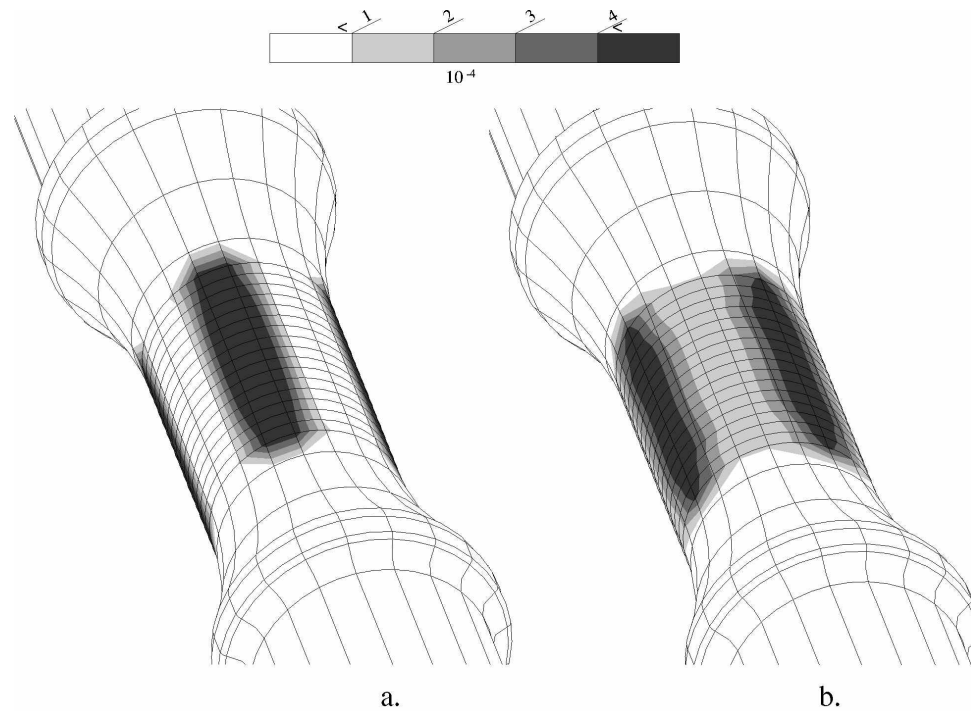
Strain gauges response in pure torsion

Yield surface determined on the single crystal tube



Note that Hill's criterion give wrong results

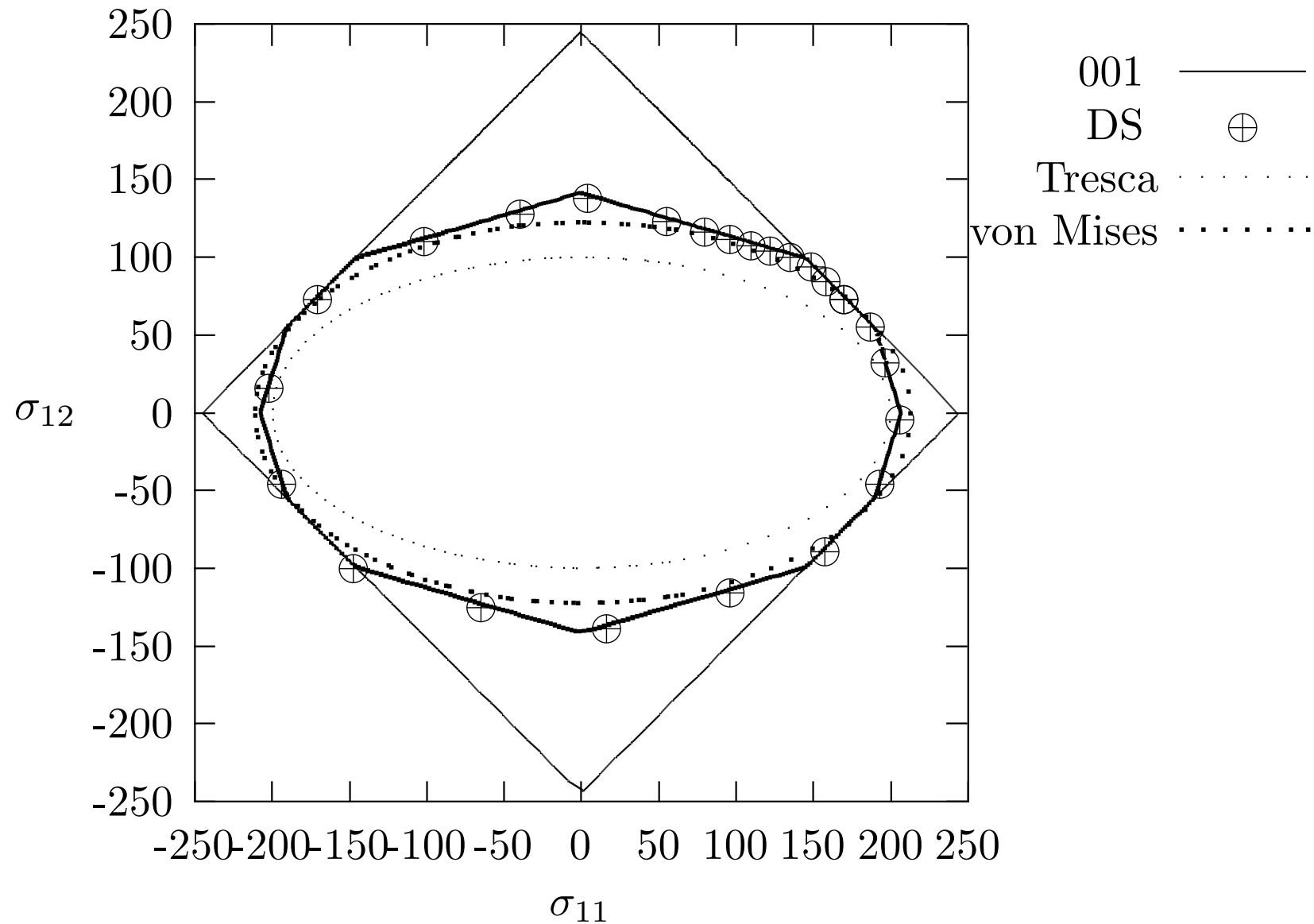
Location of the soft zones for different ratio tension/torsion on the tube



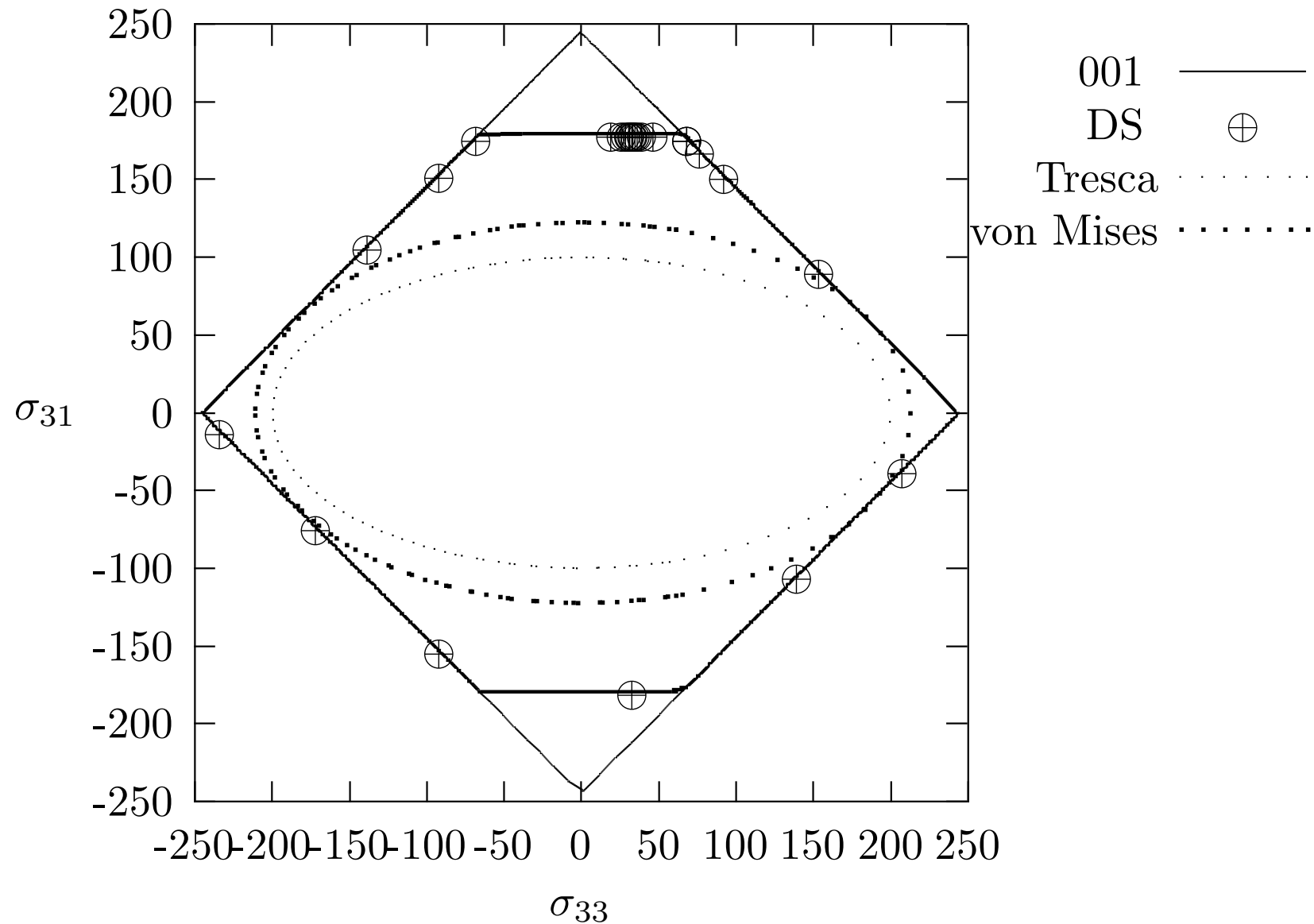
Loading surface of a directionally solidified material

- 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.
- In the plane $\sigma_{11}-\sigma_{12}$, the large number of systems produces a Tresca like criterion
- In the plane $\sigma_{33}-\sigma_{13}$, no new possibility, then the surface keeps angles

Yield surface for DS material with 3 orientations



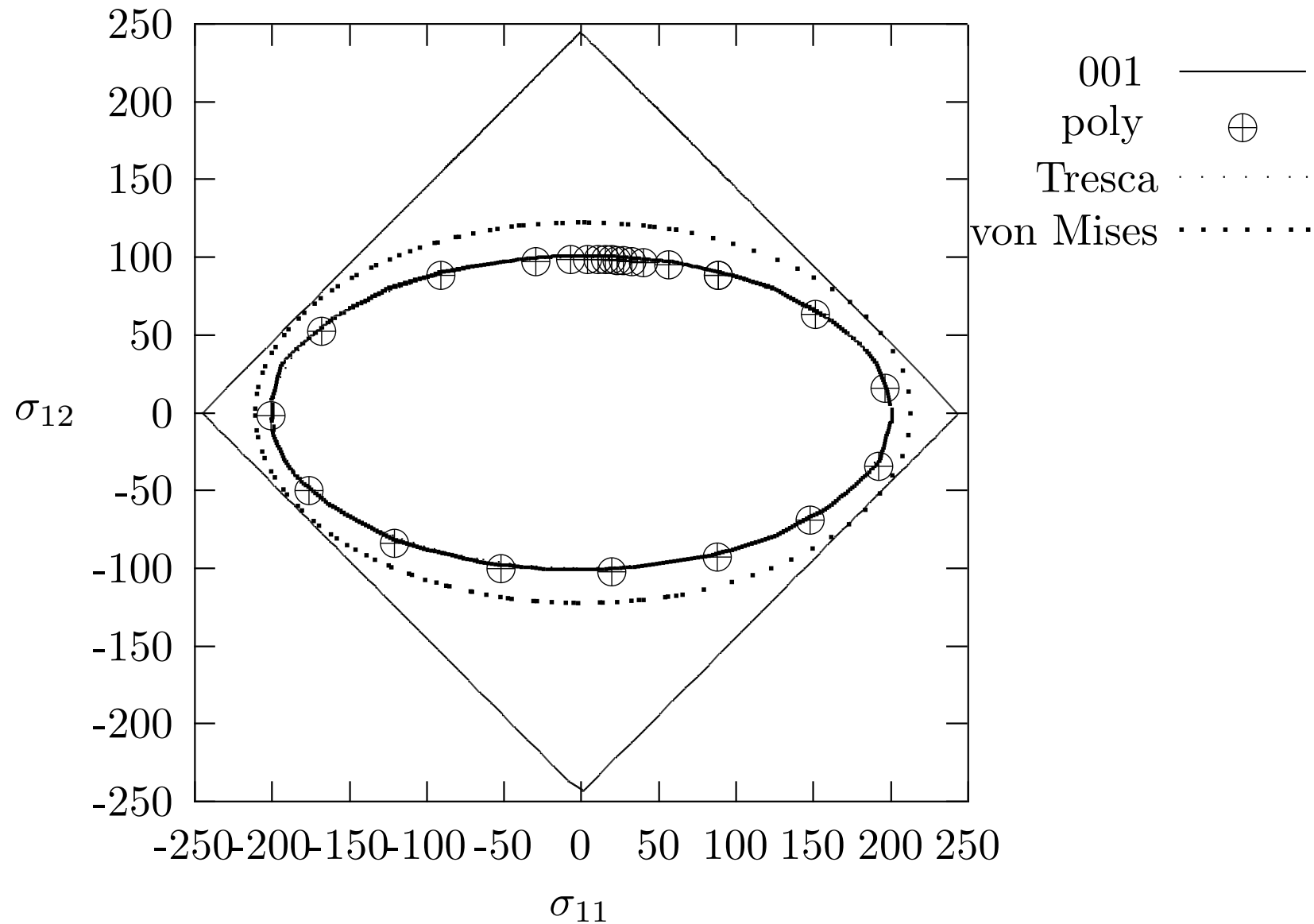
Yield surface for DS material with 3 orientations



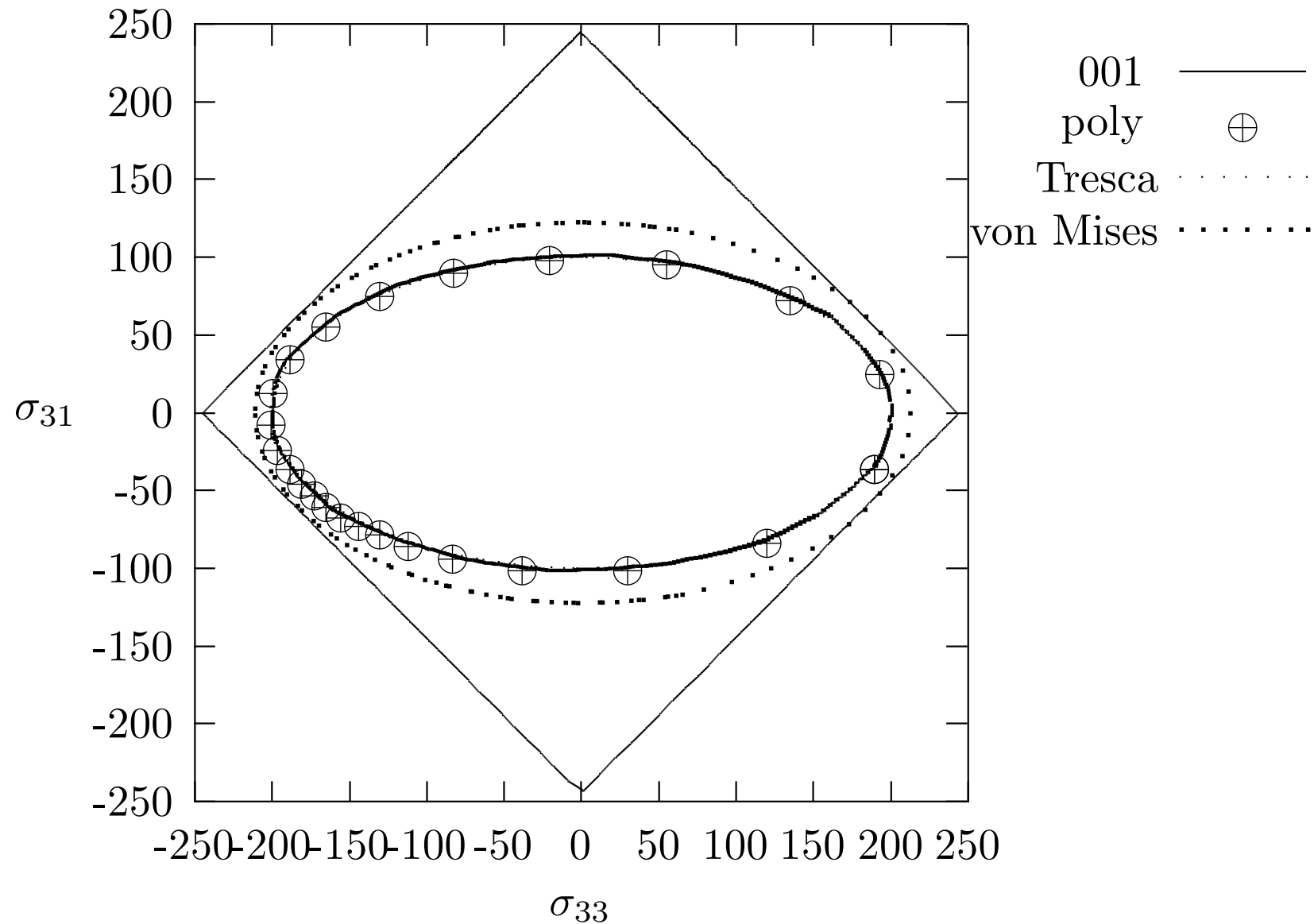
Loading surface of a polycrystalline material

- The orientation of a grain is defined by a set of three Euler angles, (ϕ_1, Φ, ϕ_2)
- Assume an uniform elasticity
- Tresca like criterion is obtained for both planes $\sigma_{33}-\sigma_{13}$ and $\sigma_{11}-\sigma_{12}$

Yield surface for a polycrystalline aggregate with **100 orientations**



Yield surface for a polycrystalline aggregate with 100 orientations



Polycrystal plasticity

Alliage Cu-Zn-Al



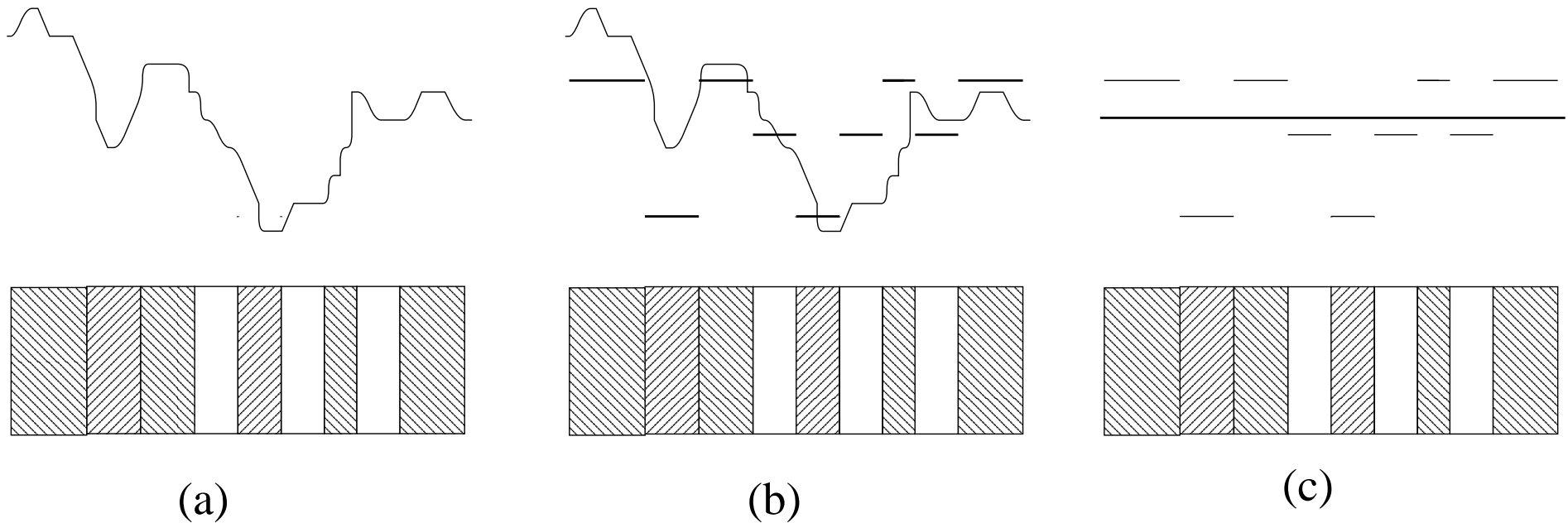
Gourgues, 1999

Various scales for behavior modeling

(a) Actual intragranular fields (*Computational Material Science*)

(b) Uniform fields in each crystallographic phase

(c) Macroscopic phenomenological models, "black box"



Introduction of a parametric scale transition rule

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

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

$$\underline{\underline{B}} = \sum_g f_g \underline{\underline{\beta}}^g$$

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

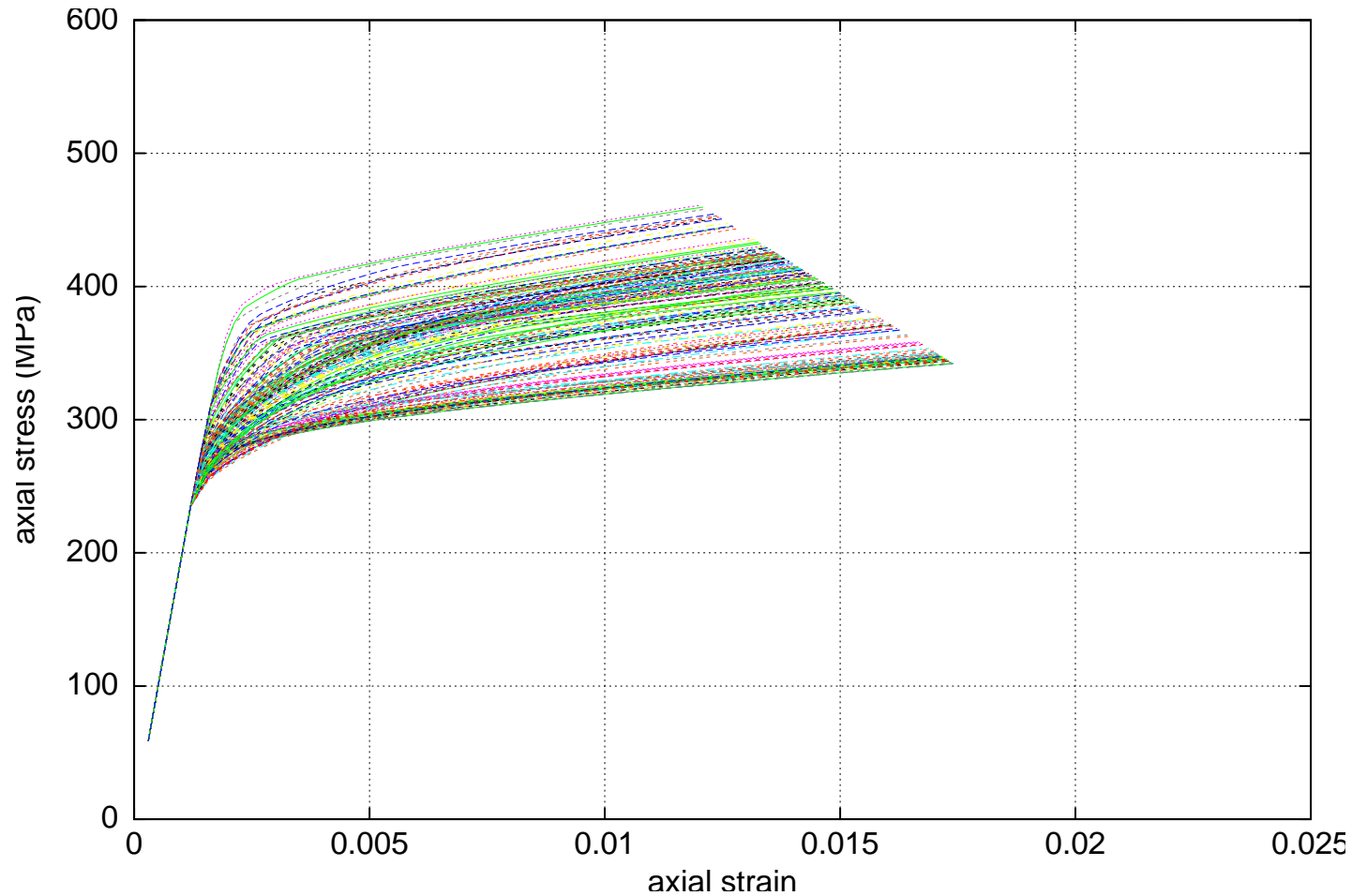
- New interphase accommodation variables $\underline{\underline{\beta}}^g$, with a kinematic evolution rule [Cailletaud 87]

- rule 1: $\dot{\underline{\underline{\beta}}}^g = \dot{\underline{\underline{\xi}}}^g - D \dot{\underline{\underline{\epsilon}}}_{eq}^g \underline{\underline{\beta}}^g$

- rule 2: $\dot{\underline{\underline{\beta}}}^g = \dot{\underline{\underline{\xi}}}^g - D \dot{\underline{\underline{\epsilon}}}_{eq}^g (\underline{\underline{\beta}}^g - \delta \underline{\underline{\xi}}^g)$

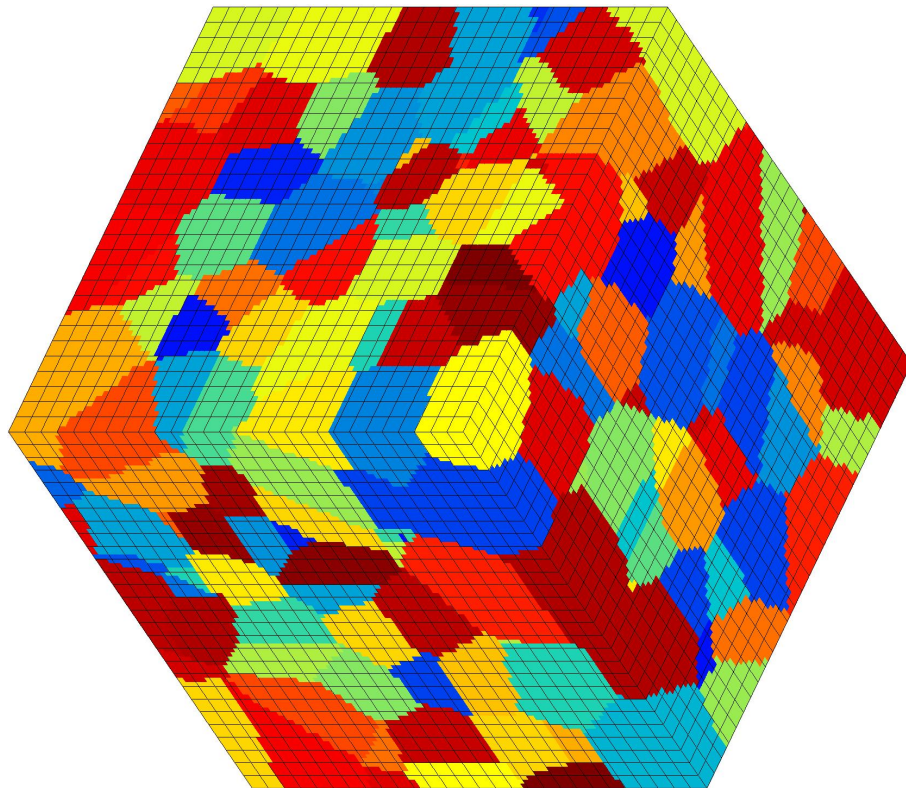
- Identification procedure, inverse approach from finite element [Pilvin 97]: the coefficient C , D , δ , are not exactly material coefficients, but *scale transition parameters*, which should be fitted from Finite Element computation on realistic polycrystalline aggregates.

Physical meaning of the transition rule

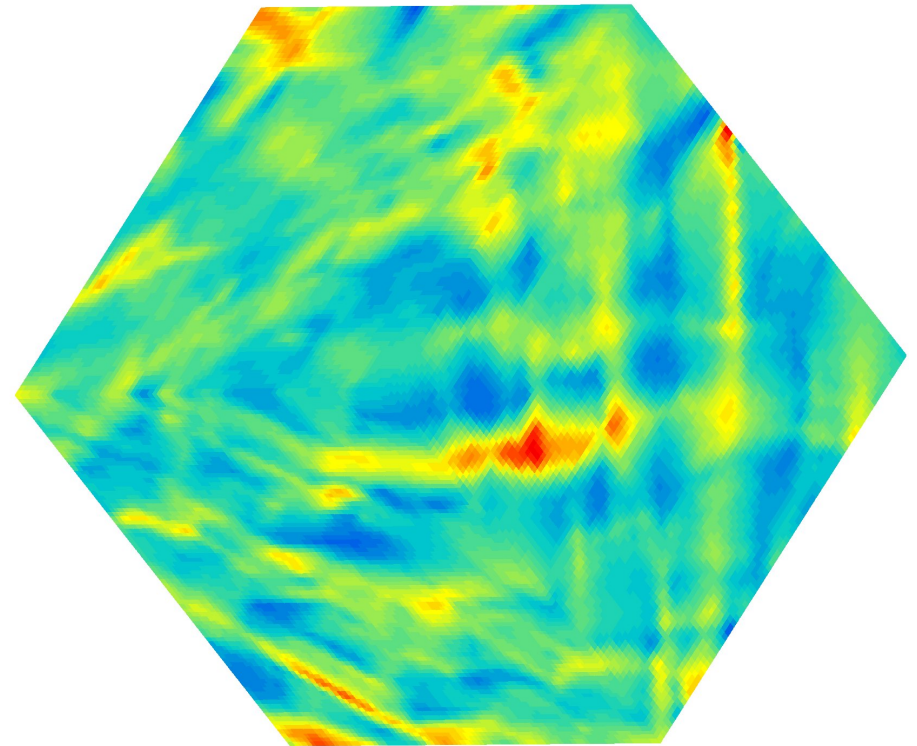


If $D = 0$, $C = \mu$: Kröner's rule; if $C = 0$: static model; if $C \rightarrow \infty$: Taylor model

An example on microstructure calculation: axial strain field

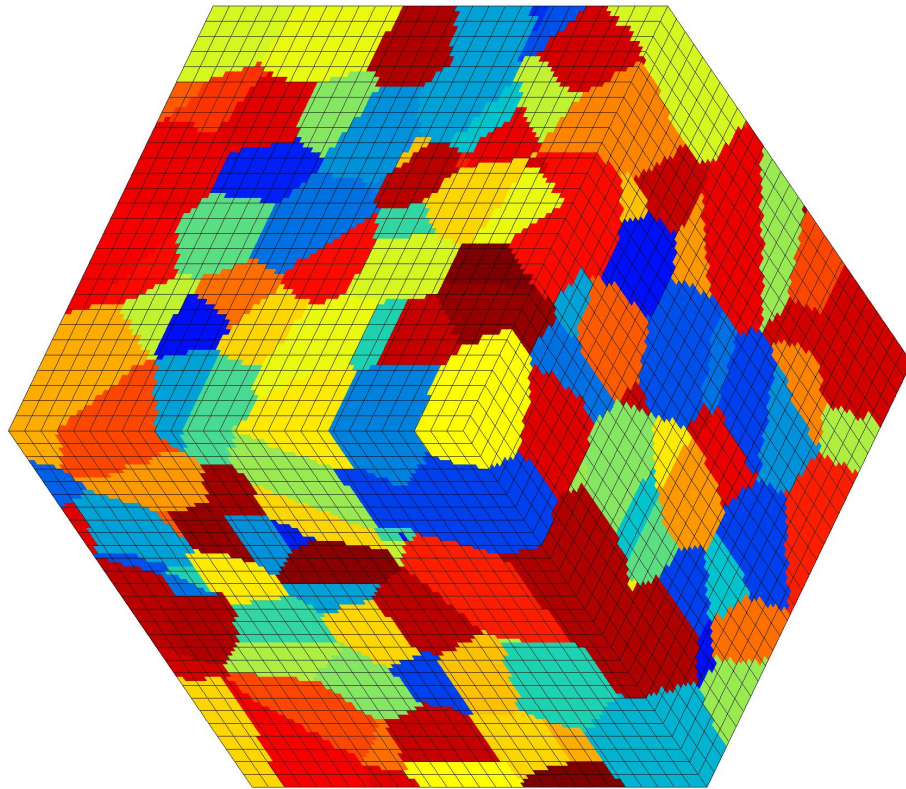


28x28x28 mesh

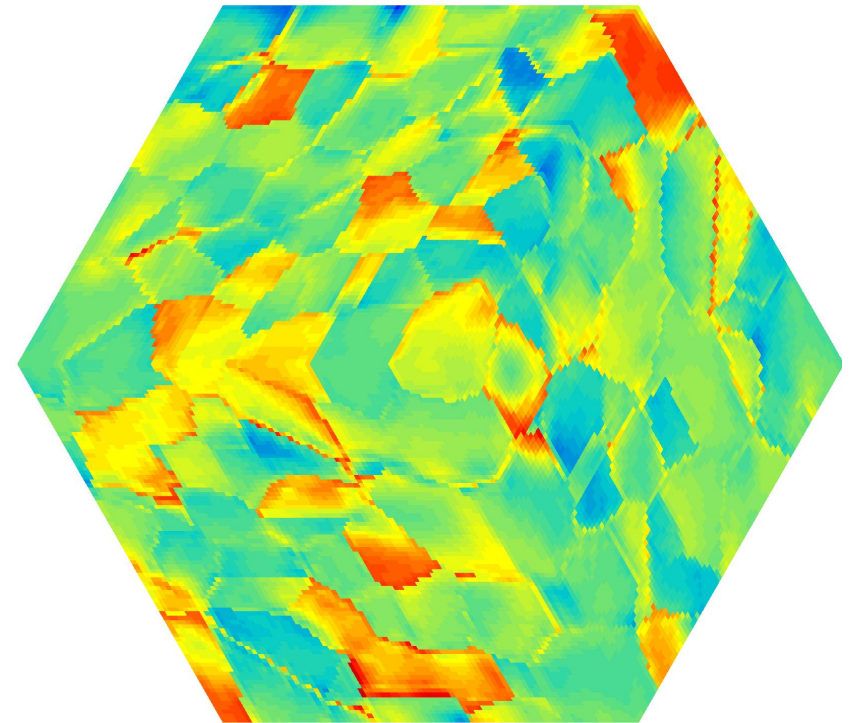


Deformation localization along bands

An example on microstructure calculation: von Mises stress field



28x28x28 mesh



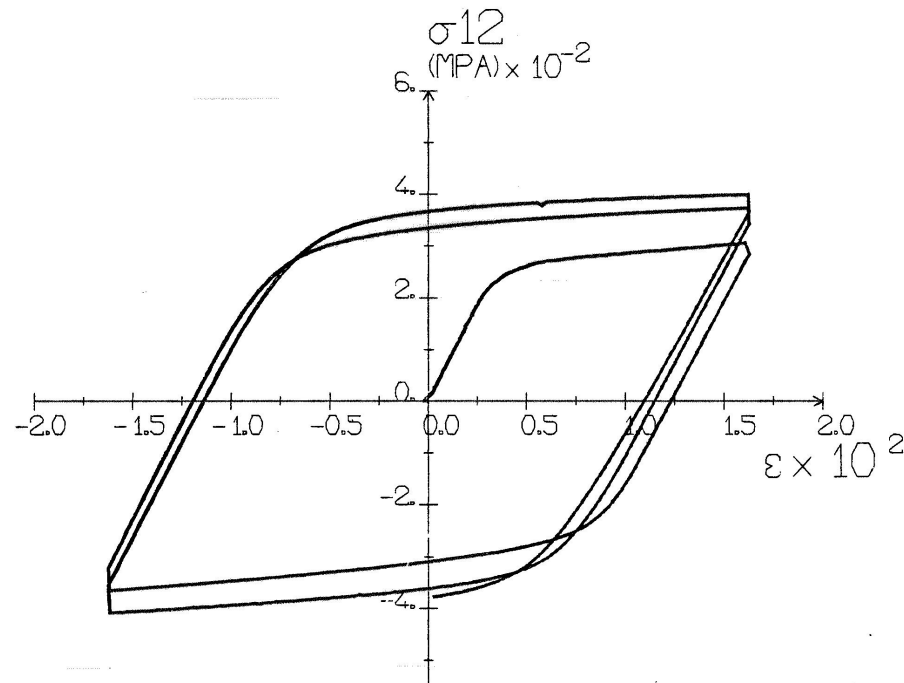
Stress heterogeneities respect grain boundaries

Main features of the polycrystal models

- Initial texture, texture evolution
- Distorsion of yield surface
- Strain memory effect
- Additional hardening
- Ratchetting

Distorsion of a yield surface (1)

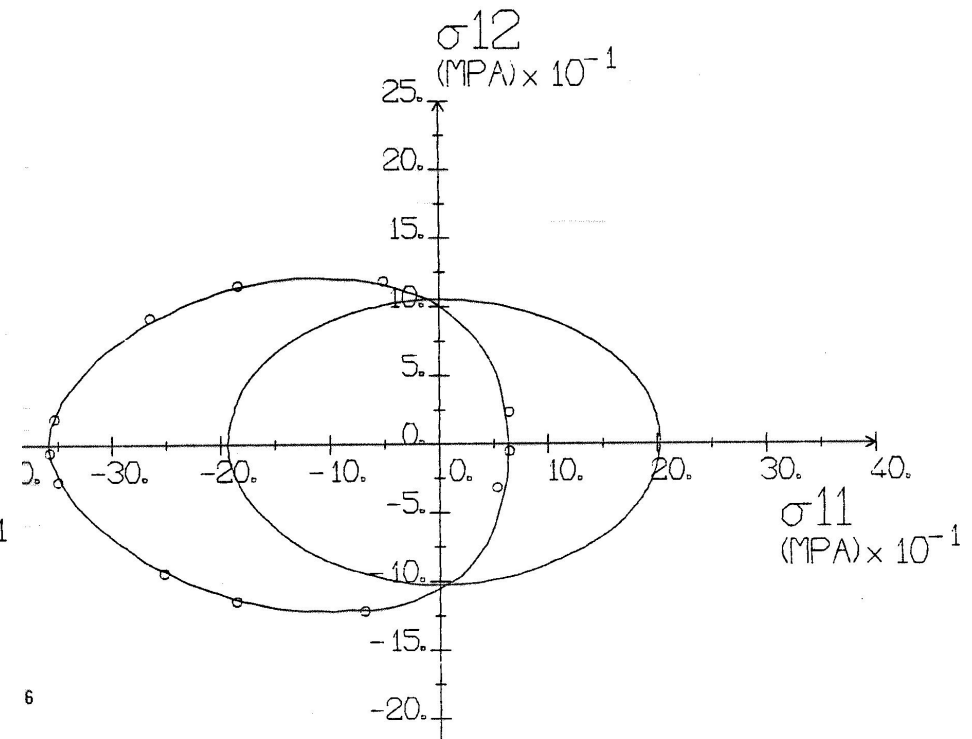
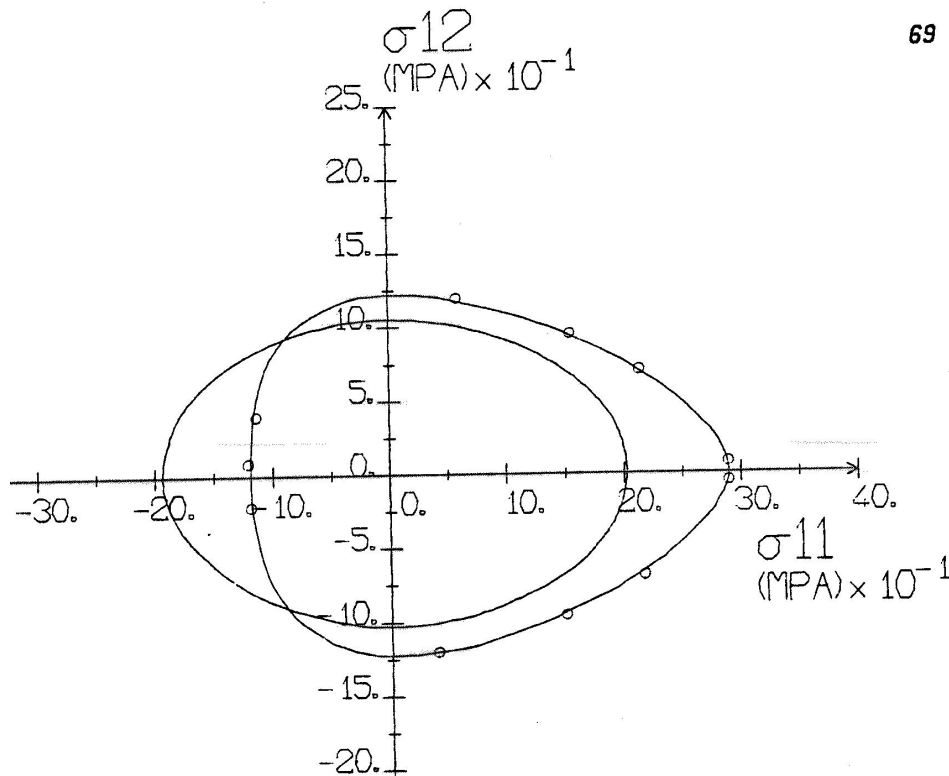
Fatigue tests on a 2024 aluminium alloy



PhD Marc Rousset, 1985

Experimental distortion of a yield surface (2)

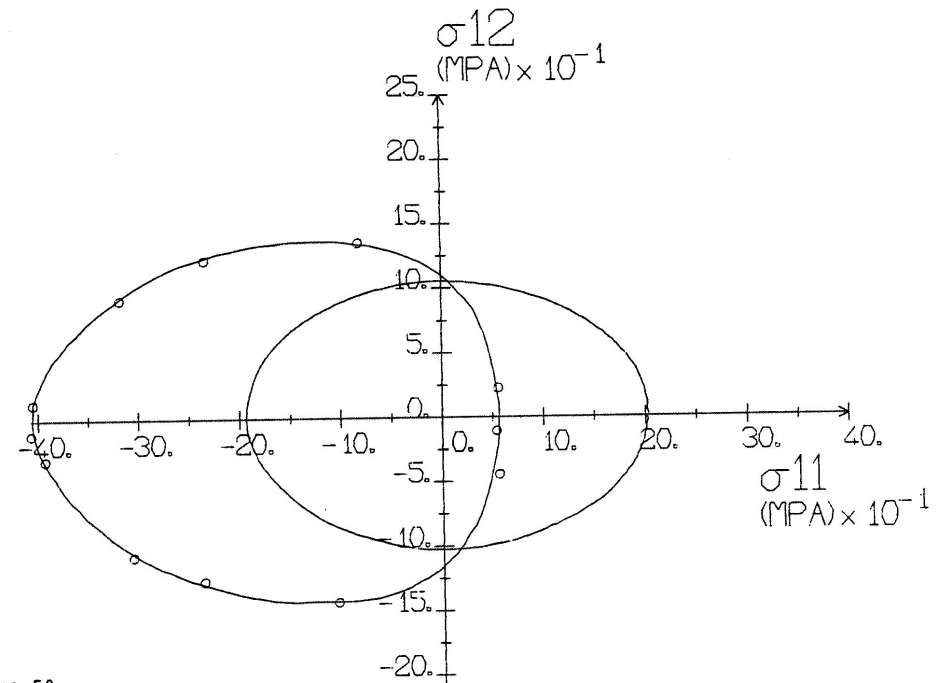
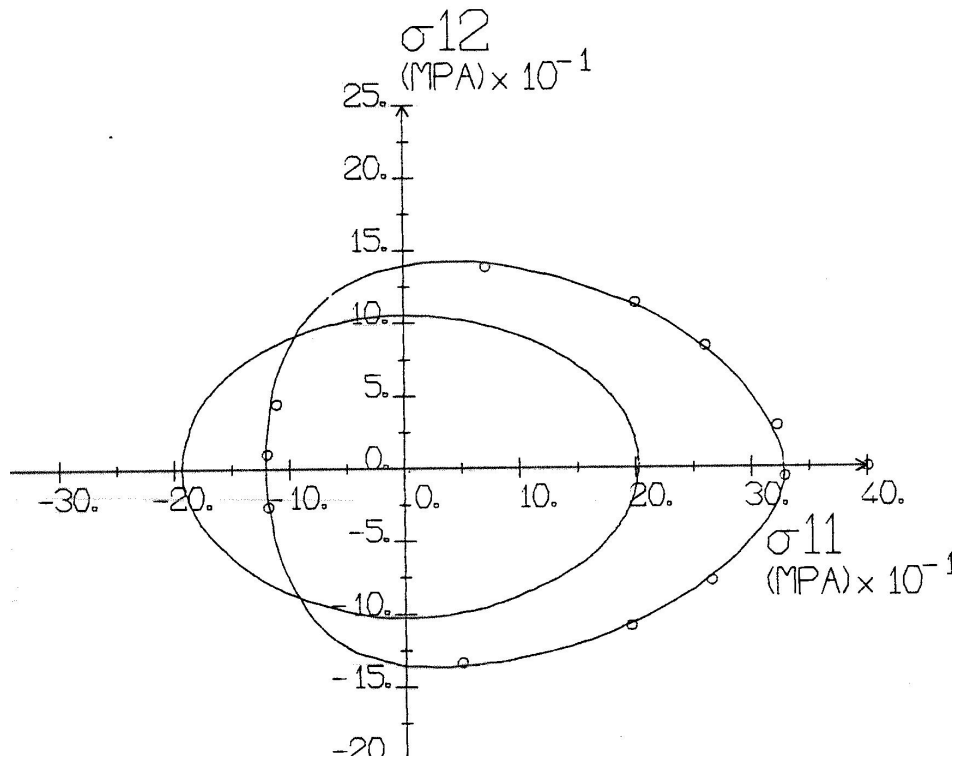
First cycle



PhD Marc Rousset, 1985

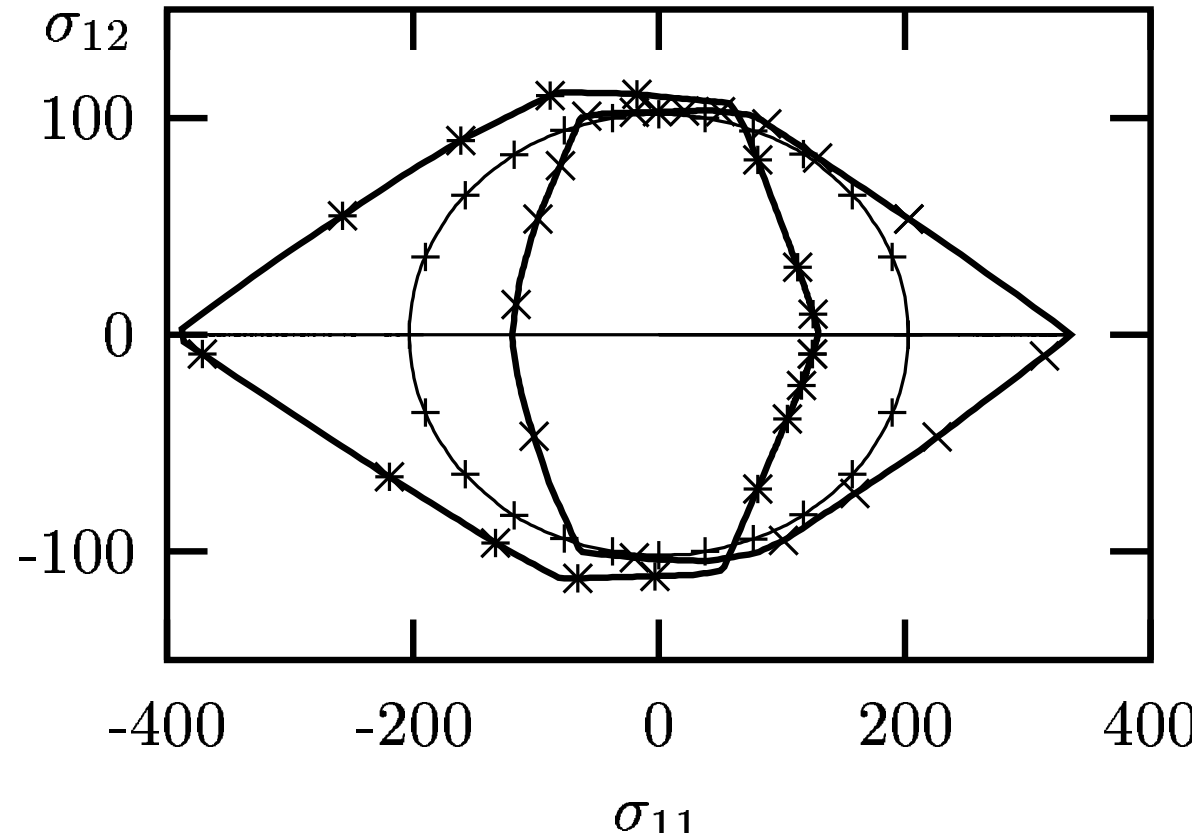
Experimental distortion of a yield surface (3)

Second cycle



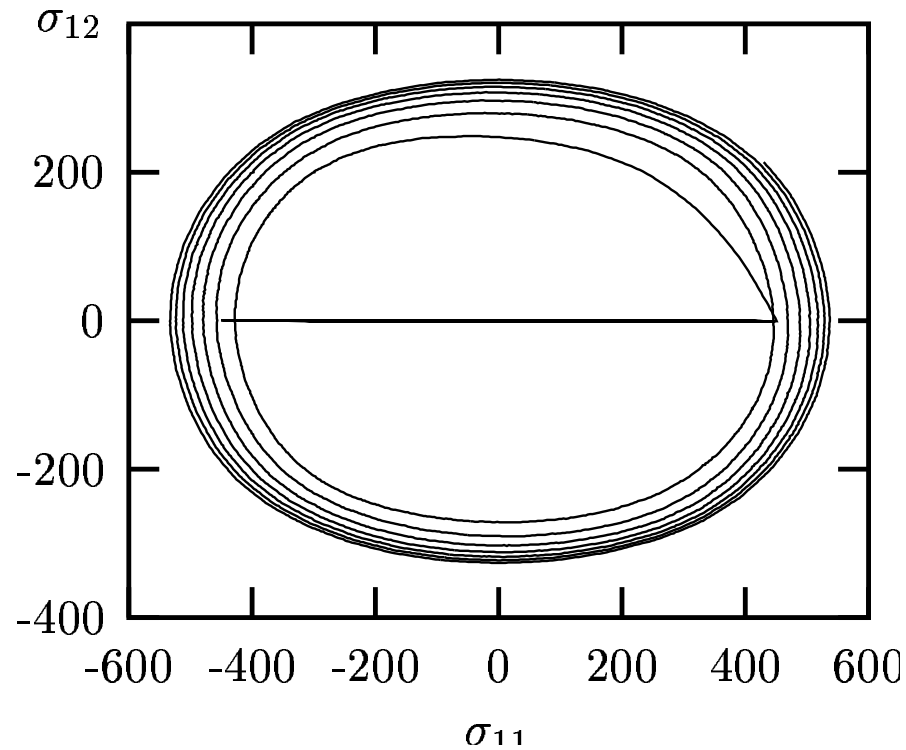
PhD Marc Rousset, 1985

Distorsion of a yield surface during a fatigue test: simulation

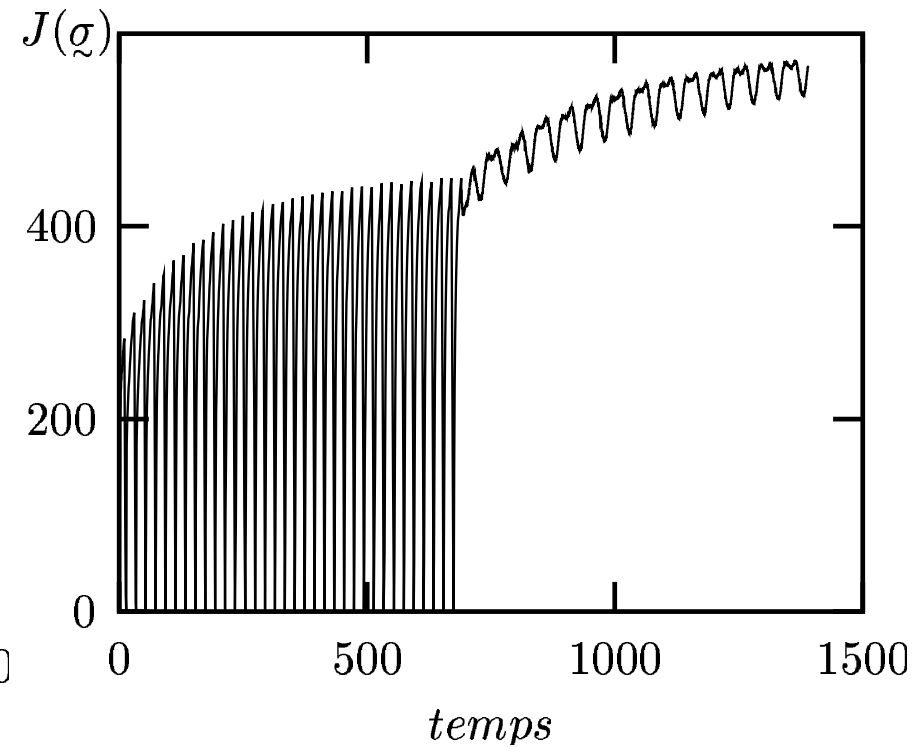


Good modeling of the corner effect

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



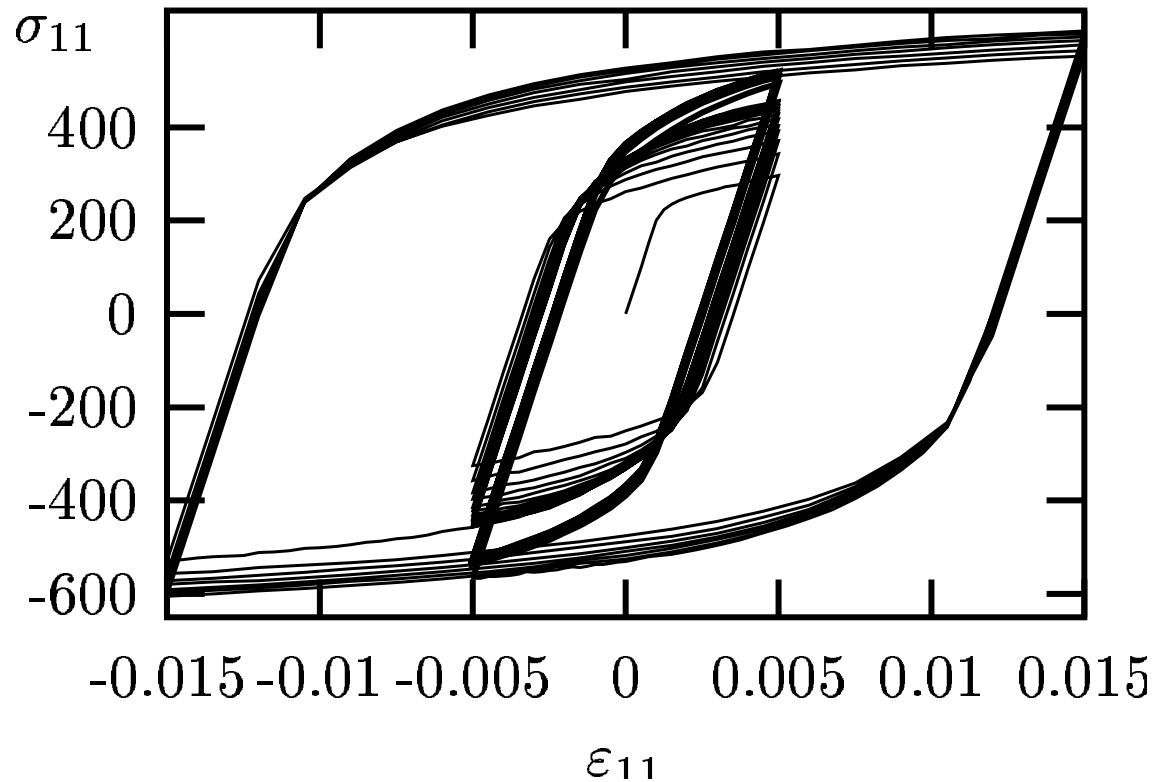
Response in the stress plane



Evolution of the equivalent stress

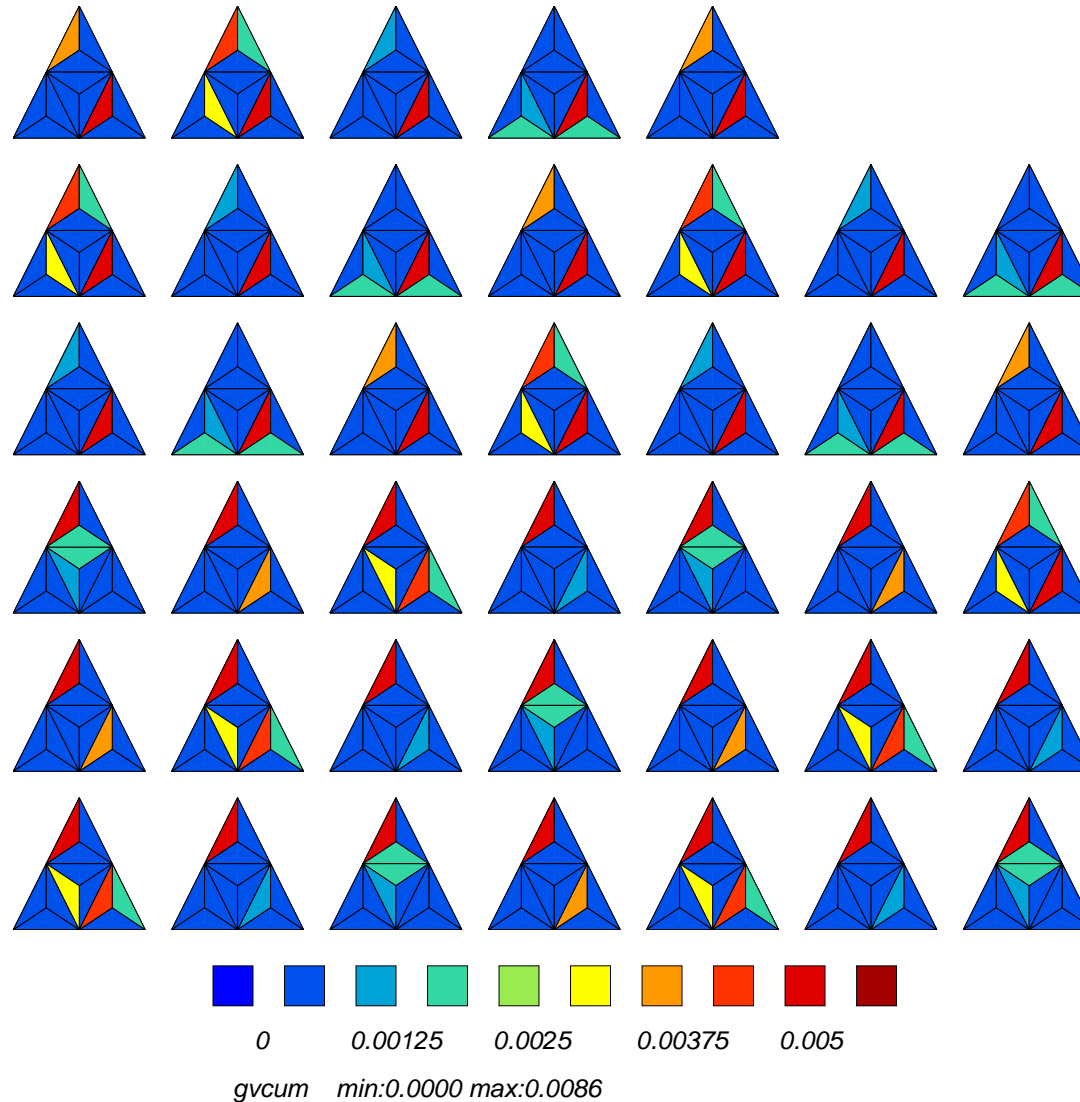
The loading is a circle in $\varepsilon_{11}-\varepsilon_{12}$ plane

Simulation of the memory effect



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

Contour of accumulated slip after a tension test



Multisurface models, crystal plasticity



- **Models using von Mises type criteria maybe convenient, specially for controlling creep-plasticity coupling**
- **Crystal plasticity for single crystal is operational**
- **Crystal plasticity for polycrystal is useful for understanding the local behavior**

–Review alternative modeling routes–