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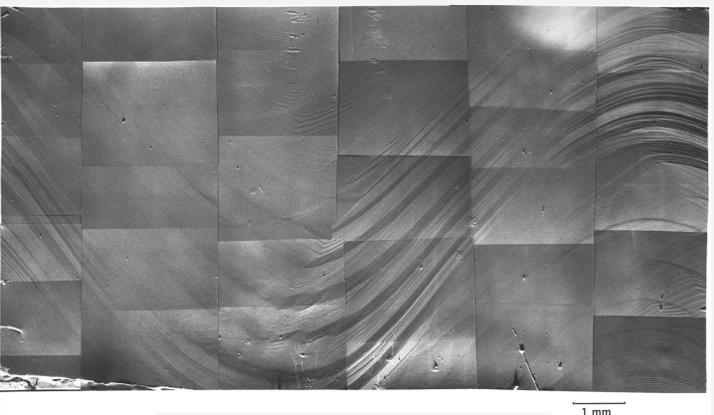
An introduction to single crystal plasticity

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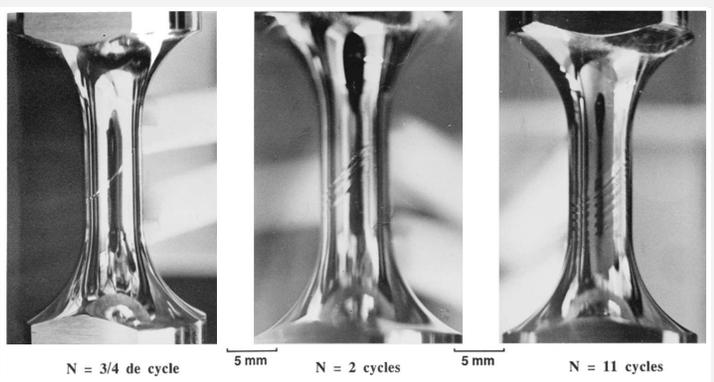
"Nul plus haut enseignement artistique ne me paraît pouvoir être reçu que du cristal"
André Breton, L'amour fou

Replica of a tensile single crystal specimens



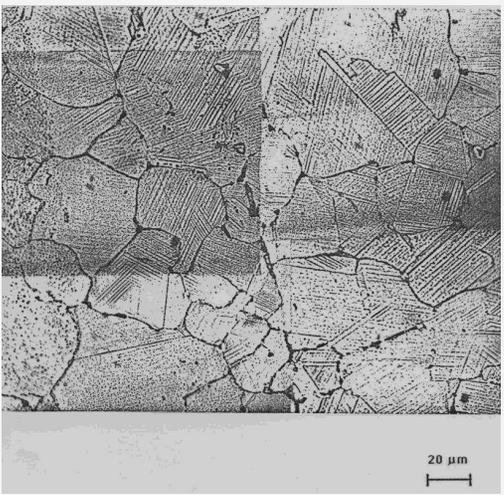
Initial yield (PhD F.Hanriot, 1993)

Single crystal specimens



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

Polycrystal specimens



Slip systems in waspaloy (M. Clavel, 1978)

Thermodynamics: first principle

- First principle, using internal energy on a domain \mathcal{D} , E , and specific internal energy, e

$$\frac{dE}{dt} = \int_{\mathcal{D}} \rho \frac{de}{dt} dV = \mathcal{P}^{(e)} + \dot{Q}$$

- Power of external forces

$$\mathcal{P}^{(e)} = \int_{\mathcal{D}} \underline{\sigma} : \underline{\dot{\epsilon}} dV$$

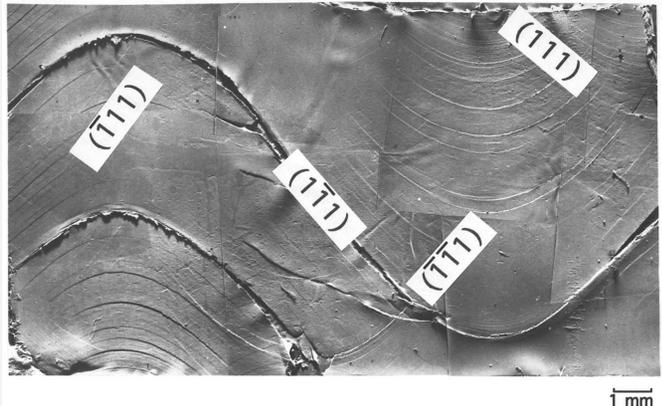
- Heat exchanged, using the rate of captured heat, \underline{q} , and \underline{n} , outside normal to the surface $\partial\mathcal{D}$, and r , volumetric heat

$$\dot{Q} = \int_{\mathcal{D}} r dV - \int_{\partial\mathcal{D}} \underline{q} \cdot \underline{n} dS = \int_{\mathcal{D}} (r - \text{div}\underline{q}) dV$$

- Variation of internal energy

$$\rho \frac{de}{dt} = \underline{\sigma} : \underline{\dot{\epsilon}} + r - \text{div}\underline{q}$$

Replica of a tensile single crystal specimens (2)



End of life (PhD F.Hanriot, 1993)

Polycrystal specimens



Cu-Zn-Al (F. Gourgues, 1999)

Dissipation

- Application of the method of local state: Ψ depends on temperature and state variables α_i

$$\frac{d\Psi}{dt} = \frac{\partial\Psi}{\partial T} \dot{T} + \frac{\partial\Psi}{\partial\alpha_i} \dot{\alpha}_i$$

$$s = -\frac{\partial\Psi}{\partial T}$$

$$\sigma_{ij} \dot{\epsilon}_{ij} - \rho \frac{\partial\Psi}{\partial\alpha_i} \dot{\alpha}_i - \frac{1}{T} \mathbf{q} \cdot \mathbf{grad}(T) \geq 0 \quad (4)$$

- Intrinsic dissipation Φ_1 , thermal dissipation Φ_2 :

$$\Phi_1 = \sigma_{ij} \dot{\epsilon}_{ij} - \rho \frac{\partial\Psi}{\partial\alpha_i} \dot{\alpha}_i \quad \Phi_2 = -\frac{1}{T} \mathbf{q} \cdot \mathbf{grad}(T)$$

Thermodynamics: second principle

The second principle provides a superior bound of the heat rate received by the volume \mathcal{D} at a temperature T , and can be expressed as a function of the entropy S or of the specific entropy s :

$$\frac{dS}{dt} \geq \int_{\mathcal{D}} \frac{r}{T} dV - \int_{\partial\mathcal{D}} \frac{\mathbf{q} \cdot \mathbf{n}}{T} dS$$

d'où :

$$\int_{\mathcal{D}} \left(\rho \frac{ds}{dt} - \frac{r}{T} + \text{div} \left(\frac{\mathbf{q}}{T} \right) \right) dV \geq 0$$

Using Helmholtz free energy Ψ , such as $e = \Psi + Ts$, one get the so called Clausius-Duhem inequality

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}} - \rho \frac{d\Psi}{dt} - \rho s \dot{T} - \frac{1}{T} \mathbf{q} \cdot \mathbf{grad}(T) \geq 0$$

Thermo-elasticity (1)

- Zero elastic strain for $\boldsymbol{\sigma}^I$, zero thermal strain for T^I
- The state variable is elastic strain: $\alpha_i \equiv \epsilon^e$ in intrinsic dissipation
- No dissipation for an elastic isothermal perturbation around equilibrium, then

$$\Phi_1 = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^e - \rho \frac{\partial\Psi}{\partial\boldsymbol{\epsilon}^e} : \dot{\boldsymbol{\epsilon}}^e = 0$$

This provides a definition for stress.

- Two state variables, two energetically conjugated variables:

State variable	Conjugated variable
T	entropy $s = -\frac{\partial\Psi}{\partial T}$
$\boldsymbol{\epsilon}^e$	stress $\boldsymbol{\sigma} = \frac{\partial\Psi}{\partial\boldsymbol{\epsilon}^e}$

Ψ is a thermodynamic potential characterizing reversible processes

Heat equation

- Decoupling of intrinsic and thermal dissipations, each of them must be positive
- Fourier's law :

$$\mathbf{q} = -k(T, \alpha_i) \mathbf{grad}(T)$$

- Heat equation in presence of mechanical strain:

$$\text{div} (k \mathbf{grad}(T)) = \rho C_\epsilon \dot{T} - r - \sigma_{ij} \dot{\epsilon}_{ij} + \rho \left(\frac{\partial\Psi}{\partial\alpha_i} - T \frac{\partial^2\Psi}{\partial T \partial\alpha_i} \right) \dot{\alpha}_i \quad (5)$$

(with $C_\epsilon = T \frac{\partial s}{\partial T}$, specific heat at a constant deformation)

Temperature changes for elastic loadings

Temperature variation related to volume change:

$$(T - T') = -\frac{3K\alpha T'}{\rho C_\epsilon} \epsilon_{II}^e$$

Cooling during tension

Loading curves

— isothermal : $\sigma - \sigma' = \lambda \text{Tr} \underline{\underline{\epsilon}}^e \mathbf{1} + 2\mu \underline{\underline{\epsilon}}^e$

— adiabatic : $\sigma - \sigma' = \left(\lambda + \frac{9K^2\alpha^2 T'}{\rho C_\epsilon} \right) \text{Tr} \underline{\underline{\epsilon}}^e \mathbf{1} + 2\mu \underline{\underline{\epsilon}}^e$

No change on shear modulus, variation of the axial component

Standard models (1)

- A model is standard if one can find a potential $\Omega \equiv \Omega(Z)$ such as:

$$\dot{z} = \frac{\partial \Omega}{\partial Z}$$

- If Ω is a convex function of Z which includes the origin, the dissipation is automatically positive, since:

$$\phi_1 = Z \frac{\partial \Omega}{\partial Z}$$

(all the points of the surface Ω are on the same side of the tangent plane defined by $\frac{\partial \Omega}{\partial Z}$)

- One can also define (through the Legendre-Fenchel transform) a companion potential in terms of \dot{z} :

$$\Omega^*(\dot{z}) = \max_Z (Z\dot{z} - \Omega(Z))$$

- A new potential, expressed as $\Omega^*(\dot{z})$ or $\Omega(Z)$ must be introduced to characterize the dissipative processes.

Thermo-elasticity (2)

Assume the following form for free energy:

$$\rho \Psi = \sigma' : \underline{\underline{\epsilon}}^e + \frac{1}{2} \lambda (\text{Tr} \underline{\underline{\epsilon}}^e)^2 + \mu \underline{\underline{\epsilon}}^e : \underline{\underline{\epsilon}}^e - 3K\alpha \text{Tr} \underline{\underline{\epsilon}}^e (T - T') - \frac{1}{2} \frac{\rho C_\epsilon}{T'} (T - T')^2$$

The stress is then:

$$\sigma = \rho \frac{\partial \Psi}{\partial \underline{\underline{\epsilon}}^e} = \sigma' + \lambda \text{Tr} \underline{\underline{\epsilon}}^e \mathbf{1} + 2\mu \underline{\underline{\epsilon}}^e - 3K\alpha (T - T') \mathbf{1}$$

$$\sigma - \sigma' = \lambda (\text{Tr} \underline{\underline{\epsilon}}^e - 3\alpha (T - T')) \mathbf{1} + 2\mu \underline{\underline{\epsilon}}^e$$

Variation of specific entropy:

$$\rho s = -\rho \frac{\partial \Psi}{\partial T} = 3K\alpha \text{Tr} \underline{\underline{\epsilon}}^e + \frac{\rho C_\epsilon}{T'} (T - T')$$

Application to dissipative processes

- Definition of state variables α_I and of hardening variables A_I

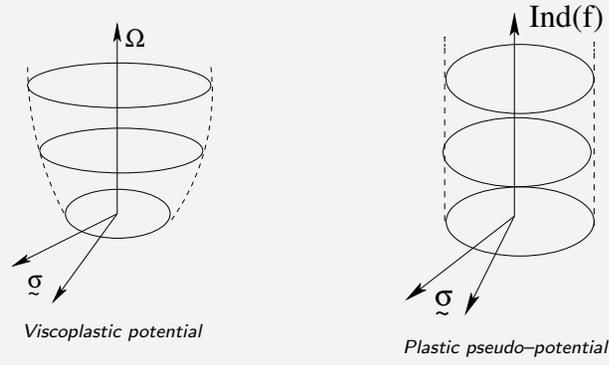
State variable	Conjugated variable	
T	$s = -\frac{\partial \Psi}{\partial T}$	entropy
$\underline{\underline{\epsilon}}^e$	$\sigma = \rho \frac{\partial \Psi}{\partial \underline{\underline{\epsilon}}^e}$	stress
α_I	$A_I = \rho \frac{\partial \Psi}{\partial \alpha_I}$	state variables

- The intrinsic dissipation can be rewritten:

$$\Phi_1 = \sigma : \underline{\underline{\dot{\epsilon}}}^p - A_I \dot{\alpha}_I = Z \dot{z}$$

with : $Z = \{\sigma, A_I\}$; $z = \{\underline{\underline{\epsilon}}^p, -\alpha_I\}$

From viscoplasticity to plasticity



- Viscoplasticity = strain rate totally defined by the potential
- Plasticity = Consistency condition needed to define strain rate intensity

Structure of a plastic model

- Let us define $\mathbb{F}(Z) = Zz - \dot{\lambda} f$ and search for the zero of $\partial \mathbb{F} / \partial Z$

$$\dot{z} = \dot{\lambda} \frac{\partial f}{\partial Z} \quad \text{then:} \quad \dot{\xi}^P = \dot{\lambda} \frac{\partial f}{\partial \sigma} = \dot{\lambda} \mathbf{n} \quad ; \quad \dot{\alpha}_I = -\dot{\lambda} \frac{\partial f}{\partial A_I}$$

- $\dot{\lambda}$ (at first unknown) plays in plasticity the rôle of the equivalent strain rate in viscoplasticity

Operational way for material model development

- Define a set of two potentials, Ψ, Ω
- Derive the relation between state variables and hardening variables from Ψ
- Derive the nature of the hardening variables and their evolution rules from Ω

In the following, example of isotropic and kinematic nonlinear hardenings; the choice for the sets (A_I, α_I) is:

Type of hardening	State variable	Conjugated variable
Isotropic hardening	r	R
Kinematic hardening	α	\mathbf{X}

NOTE: Previously, p for isotropic hardening, ξ^P for linear kinematic hardening

Plasticity framework

- Hill's "principle" (no hardening) The real stress field provides a maximum of the intrinsic dissipated power $\Phi_1 = \sigma^* : \dot{\xi}^P$ of any admissible stress field:

$$\forall \sigma^* \text{ admissible } (\sigma - \sigma^*) : \dot{\xi}^P \geq 0$$

- With hardening

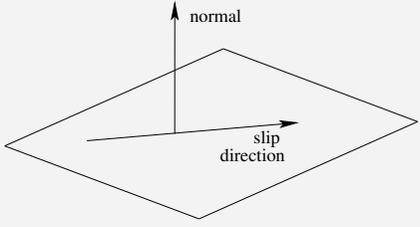
$$\Phi_1 = \sigma^* : \dot{\xi}^P - A_I^* \dot{\alpha}_I = \sigma : \dot{\xi}^P - \dot{\Psi}_p = Z \dot{z} \quad \text{maximum}$$

With Z including stress and the hardening variables A_I , z including plastic strain and the state variables $(-\alpha_I)$:

$$(Z - Z^*) \dot{z} \geq 0$$

- The maximization of Φ_1 under the constraint $f \leq 0$ can be seen as an extension of Hill's principle.

Basic ingredients of crystal plasticity



- A collection of N slip systems
- Normal to slip plane \underline{n}^s
- Direction of slip system \underline{l}^s
- Orientation tensor

$$\underline{m}^s = \frac{1}{2}(\underline{n}^s \otimes \underline{l}^s + \underline{l}^s \otimes \underline{n}^s)$$

- Resolved shear stress

$$\tau^s = \underline{\sigma} : \underline{m}^s$$

- (Visco)plastic strain rate

$$\underline{\dot{\epsilon}}^p = \sum_s \dot{\gamma}^s \underline{m}^s$$

- One yield function, f^s , for each system

- (Visco)plastic flow

$$\dot{\gamma}^s = \Phi(f^r) \quad \text{or ...}$$

$$\dot{\gamma}^s = \Phi((f^r, \dot{r}^r))$$

Free energy

- Elasticity (non-dissipative process) is fully defined as

$$\rho\psi^e = \frac{1}{2} \underline{\underline{\xi}}^e : \underline{\underline{\Lambda}} : \underline{\underline{\xi}}^e$$

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

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

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

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

- Note the interaction matrix, whose components h_{rs} characterize self-hardening (if $r = s$) and cross-hardening (if $r \neq s$)

State coupling, dissipative coupling

- State coupling, in the free energy (note the symmetry of the interactions):

$$\Psi(\alpha_1, \alpha_2) = \frac{1}{2} c_{11} \alpha_1^2 + \frac{1}{2} c_{22} \alpha_2^2 + \frac{1}{2} c_{12} \alpha_1 \alpha_2$$

α_1 et α_2 :

$$\frac{\partial A_1}{\partial \alpha_2} = \frac{\partial A_2}{\partial \alpha_1} = \frac{\partial^2 \phi}{\partial \alpha_1 \partial \alpha_2}$$

- Dissipative coupling, when Ω is the sum of several potential functions, Ω_K :

$$\dot{z} = \sum_K \frac{\partial \Omega_K}{\partial Z}$$

(more in [Germain et al., 1983, Lemaitre and Chaboche, 1990, Besson et al., 1998])

State variables and hardening rules on slip systems

Phenomenon	State variable	Associated variable
Elasticity	$\underline{\underline{\xi}}^e$	$\underline{\underline{\sigma}}$
Isotropic hardening	$\rho^s, s = 1..N$	$r^s, s = 1..N$
Kinematic hardening	$\alpha^s, s = 1..N$	$x^s, s = 1..N$

- Strain partition (small strain)

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

- The relation between state and associated variables comes from free energy

$$\rho\psi(\underline{\underline{\xi}}^e, \rho^s, \alpha^s) = \rho\psi^e(\underline{\underline{\xi}}^e) + \rho\psi^p(\rho^s, \alpha^s)$$

- Viscoplasticity needs the definition of a viscoplastic potential, plasticity needs the definition of a plastic pseudopotential. They are built using the expression of the yield criterion on each slip system

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

Hardening rules

- Standard model

$$\dot{\alpha}^s = \frac{\partial \Omega}{\partial x^s} = \sum_r \frac{\partial \Omega_r}{\partial x^s} = \frac{\partial \Omega_s}{\partial f^s} \frac{\partial f^s}{\partial x^s} = \dot{v}^s \eta^s = \dot{\gamma}^s$$

$$\dot{\rho}^s = \frac{\partial \Omega}{\partial r^s} = \sum_r \frac{\partial \Omega_r}{\partial r^s} = \frac{\partial \Omega_s}{\partial f^s} \frac{\partial f^s}{\partial r^s} = \dot{v}^s$$

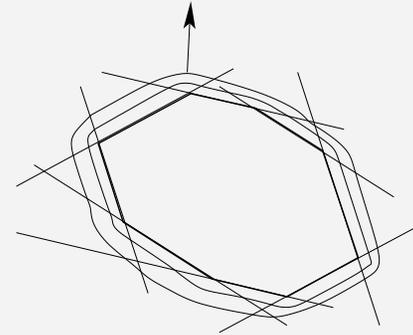
- Non standard model

$$\dot{\alpha}^s = (\eta^s - x^s) - d\alpha^s \dot{v}^s$$

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

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Anatomy of viscoplastic and plastic formulations

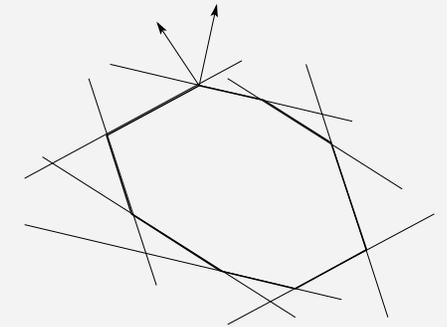


Viscoplastic potential:

$$\Omega = \sum_{s=1}^N \frac{K}{n+1} \left\langle \frac{f^s}{K} \right\rangle^{n+1}$$

$$\dot{\tilde{\epsilon}}^p = \sum_{s=1}^N \frac{\partial \Omega}{\partial f^s} \frac{\partial f^s}{\partial \tilde{\sigma}} = \sum_{s=1}^N \left\langle \frac{f^s}{K} \right\rangle^n \mathfrak{m}^s$$

Regularization of the yield surface



Plasticity

$$f^s = 0 \quad \dot{f}^s = 0$$

$$\dot{\tilde{\epsilon}}^p = \sum_{s=1}^N \dot{\lambda}^s \frac{\partial f^s}{\partial \tilde{\sigma}} = \sum_{s=1}^N \dot{\lambda}^s \mathfrak{m}^s$$

Selection of the slip systems ?

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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

$$\dot{\tilde{\epsilon}}^p = \frac{\partial \Omega}{\partial \tilde{\sigma}} = \sum_r \frac{\partial \Omega_r}{\partial \tilde{\sigma}} = \sum_r \frac{\partial \Omega_r}{\partial f^r} \frac{\partial f^r}{\partial \tilde{\sigma}} = \sum_r \dot{v}^r \mathfrak{m}^r \eta^r = \sum_r \dot{\gamma}^r \mathfrak{m}^r$$

- Characterization of shear rate

$$\frac{\partial \Omega}{\partial f^r} = \left\langle \frac{f^r}{K} \right\rangle^n = \dot{v}^r \quad \dot{\gamma}^r = \dot{v}^r \text{sign}(\tau^r - x^r) = \dot{v}^r \eta^r$$

- Normality rule

$$\frac{\partial f^r}{\partial \tilde{\sigma}} = \frac{\partial (|\mathfrak{m}^r : \tilde{\sigma} - x^r| - r^r - \tau_0)}{\partial \tilde{\sigma}} = \mathfrak{m}^r \eta^r$$

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Dissipation

- Since $\tilde{\sigma} : \dot{\tilde{\epsilon}}^p = \tilde{\sigma} : \sum_s \mathfrak{m}^s \dot{\gamma}^s = \sum_s \tilde{\sigma} : \mathfrak{m}^s \dot{\gamma}^s = \sum_s \tau^s \dot{\gamma}^s$

$$\begin{aligned} \phi_1 &= \tilde{\sigma} : \dot{\tilde{\epsilon}}^p - \sum_s x^s \dot{\alpha}^s - \sum_s r^s \dot{\rho}^s \\ &= \sum_s (\tau^s \dot{\gamma}^s - x^s (\eta^s - x^s) - d\alpha^s \dot{v}^s - r^s (1 - b\rho^s) \dot{v}^s) \\ &= \sum_s (f^s + \tau_0 + \frac{d}{c} (x^s)^2 + br^s \rho^s) \dot{v}^s \end{aligned}$$

- Viscous dissipation : $\sum_s f^s \dot{v}^s$

- Friction dissipation : $\tau_0 \sum_s \dot{v}^s$

- Dissipation due to nonlinear hardening: $\left(\frac{d}{c} (x^s)^2 + br^s \rho^s \right) \dot{v}^s$

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System to be solved for the plastic formulation

- For a given total strain rate, N equations ($N = \text{number of active slip systems}$):

$$\sum_r \left(\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\Lambda}} : \underline{\underline{\mathbf{m}}}^r + H_{sr} \right) \dot{v}^r = \underline{\underline{\mathbf{m}}}^s : \underline{\underline{\Lambda}} : \underline{\underline{\dot{\epsilon}}}$$

- Present model, non symmetric matrix:

$$\dot{x}^s = c\dot{\gamma}^s - dx^s \dot{v}^s = (c\eta^s - dx^s) \dot{v}^s = \sum_r (c\eta^r - dx^r) \delta_{rs} \dot{v}^r$$

$$\dot{r}^s = Q \sum_r bh_{sr} \exp(-bv^r) \dot{v}^r$$

$$H_{sr} = (c\eta^r - dx^r) \delta_{sr} + Qbh_{sr} \exp(-bv^r)$$

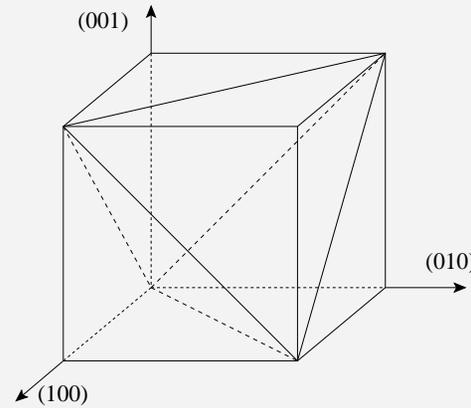
- With no kinematic hardening and linear isotropic hardening,

$$r^s = \sum_r h_{sr} v^r$$

$$H_{sr} = h_{sr}$$

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Octahedral and cubic slip systems in FCC single crystals



The four octahedral planes in a cubic crystal

Yield surfaces obtained from these definitions, using

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

- The classical slip planes in FCC alloys are 111, and the direction is 110.
- For Ni-Base superalloys, cubic planes 001 are also observed, with directions 110.

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Equations for the plastic model

- Strain partition (small strain):

$$\underline{\underline{\dot{\sigma}}} = \underline{\underline{\Lambda}} : \left(\underline{\underline{\dot{\epsilon}}} - \sum_r \underline{\underline{\mathbf{m}}}^r \dot{\gamma}^r \right)$$

- Application of the consistency condition to active slip systems:

$$f^s = |\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\sigma}} - x^s| - r^s = 0 \quad 0 = \eta^s \underline{\underline{\mathbf{m}}}^s : \underline{\underline{\dot{\sigma}}} - \eta^s \dot{x}^s - \dot{r}^s$$

using the notation $\eta^s = \text{sign}(\tau^s - x^s)$

- Compute $\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\dot{\sigma}}}$ in (2), introducing H_{sr} (see next page):

$$\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\dot{\sigma}}} = \dot{x}^s + \eta^s \dot{r}^s = \sum_r H_{sr} \dot{v}^r$$

- Then replace $\underline{\underline{\dot{\sigma}}}$ by its expression in (1):

$$\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\Lambda}} : \underline{\underline{\dot{\epsilon}}} - \sum_r \underline{\underline{\mathbf{m}}}^s : \underline{\underline{\Lambda}} : \underline{\underline{\mathbf{m}}}^r \eta^r \dot{v}^r = \sum_r H_{sr} \dot{v}^r$$

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Remark on the order of magnitude

- Note that

$$\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\mathbf{l}}} = m_{ij}^s \delta_{ij} = \text{trace}(\underline{\underline{\mathbf{m}}}^s) = m_{ii}^s = n_i^s l_i^s = 0$$

$$\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\mathbf{m}}}^s = m_{ij}^s m_{ij}^s = \frac{1}{4} (n_i^s l_j^s + l_i^s n_j^s) (n_i^s l_j^s + l_i^s n_j^s) = \frac{1}{2}$$

$$\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\mathbf{m}}}^r = m_{ij}^s m_{ij}^r = \frac{1}{4} (n_i^r l_j^r + l_i^r n_j^r) (n_i^s l_j^s + l_i^s n_j^s)$$

- Isotropic elasticity

$$\Lambda_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

$$\Lambda_{ijkl} m_{kl}^r = \mu m_{ij}^r$$

$$\underline{\underline{\mathbf{m}}}^s : \underline{\underline{\Lambda}} : \underline{\underline{\mathbf{m}}}^r = \mu m_{ij}^s m_{ij}^r$$

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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
$2\sqrt{6}m_{12}$	-1	-1	0	1	1	0	1	0	1	0	1	1
$2\sqrt{6}m_{23}$	1	0	1	-1	0	1	0	1	1	-1	1	0
$2\sqrt{6}m_{31}$	0	1	-1	0	1	1	-1	1	0	1	0	1

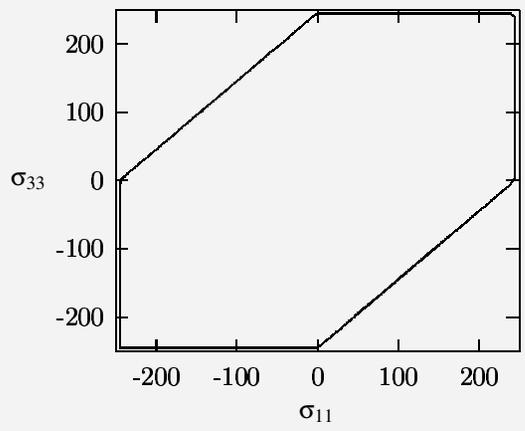
• If the only non zero terms of the stress tensor are σ_{11} , σ_{12} and σ_{21} , the criterion writes:

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

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

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

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



For biaxial tension:

- systems 1, 4, 9 and 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.

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 **n** and **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	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	1	1	0	1	0	1	0	1	1

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

For the σ_{11} and 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}

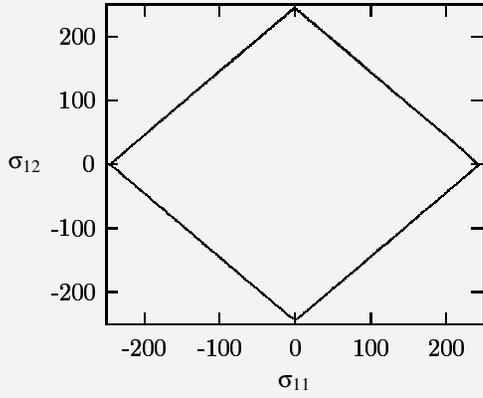
num syst	7	8	9	10	11	12
τ^s	σ_{12}	$-\sigma_{11}$	$-\sigma_{11} + \sigma_{12}$	$-\sigma_{11}$	$\sigma_{11} + \sigma_{12}$	σ_{12}

And for σ_{11} and 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 $\sigma_{11}-\sigma_{12}$ of a FCC single crystal

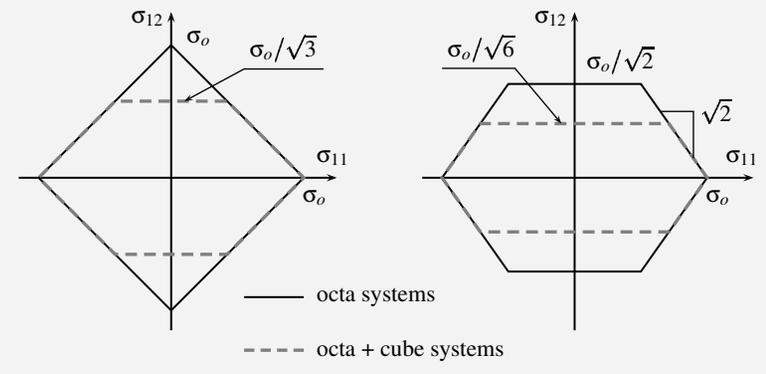


For tension–shear loading, the domain is then defined by 4 systems:

- systems 1 and 11 give : $|\sigma_{11} + \sigma_{12}| = \tau_c \sqrt{6}$
- systems 4 and 9 give : $|\sigma_{11} - \sigma_{12}| = \tau_c \sqrt{6}$

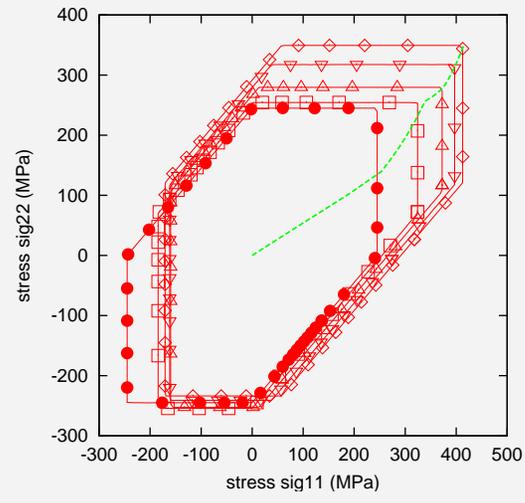
This figure is computed for $\tau_c=100$ MPa.

Influence of cubic planes on $\sigma_{11}-\sigma_{12}$ yield surface (FCC)

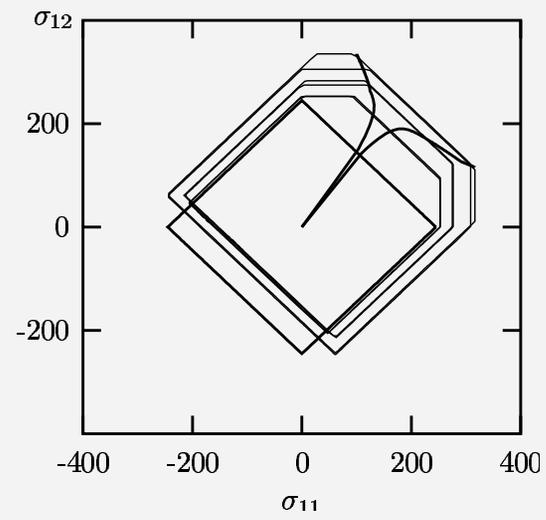


— octa systems
 - - - octa + cube systems

Subsequent evolution of the yield surfaces in $\sigma_{11}-\sigma_{22}$ plane (FCC)



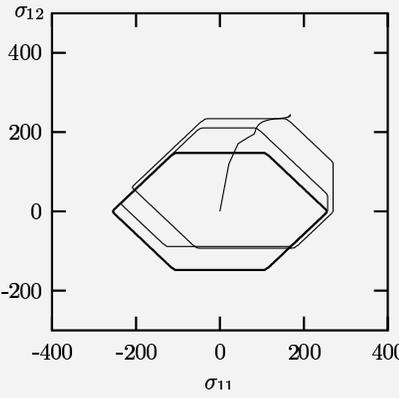
Loading path for two prescribed strain paths in 11–12 plane



- upper path: $\epsilon_{12}^{max} / \epsilon_{11}^{max} = 0,525$
- lower path: $\epsilon_{12}^{max} / \epsilon_{11}^{max} = 0,475$

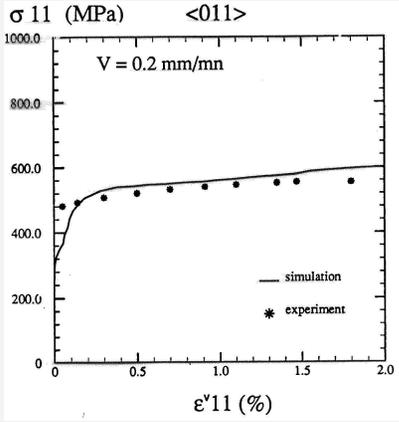
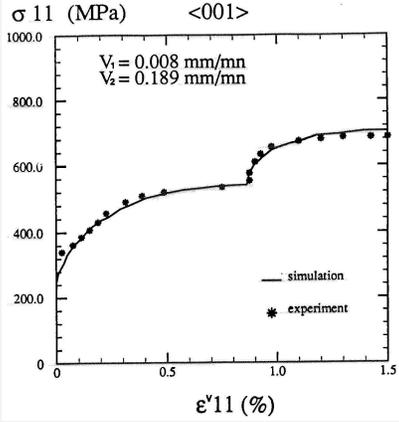
A typical example in $\sigma_{11} - \sigma_{12}$ plane

Stress response under prescribed tension–shear strain
 $\epsilon_{12} = 2\epsilon_{11}$
 Two slip system families: octahedral, cubic



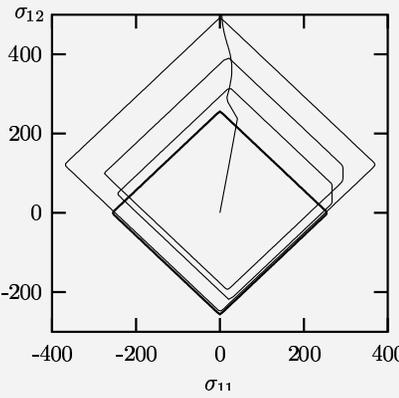
coeff (MPa,s)	octa	cube
τ_0	100	100
Q	20	10
b	10	10
c	10000	35000
d	200	700
K	20	20
n	2	2
h_{rs}	1	1

Monotonic tests on AM1 superalloy



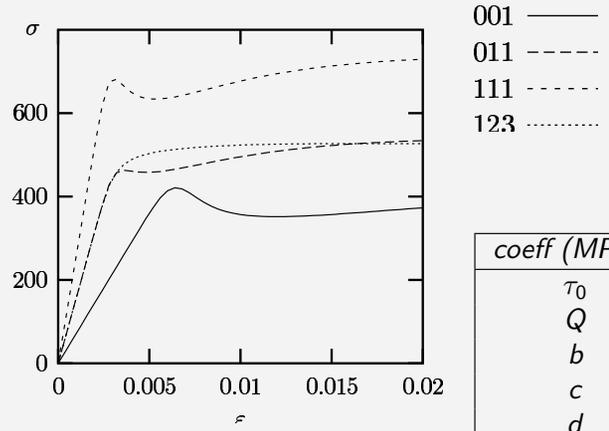
A typical example in $\sigma_{11} - \sigma_{12}$ plane

Stress response under prescribed tension–shear strain
 $\epsilon_{12} = 2\epsilon_{11}$
 One slip system family: octahedral



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_{rs}	1	1

Tensile curves for various crystallographic directions

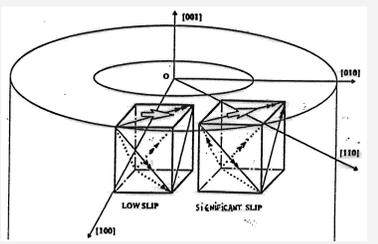
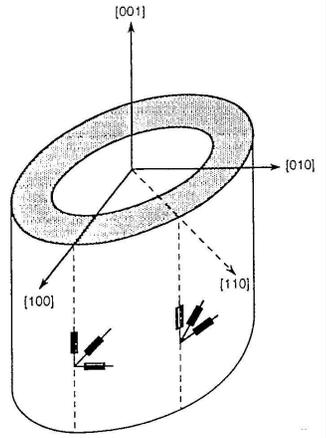


coeff (MPa,s)	syst. octa
τ_0	100
Q	-10
b	1000
c	20000
d	300
K	500
n	5
h_{ij}	1

Octahedral slip systems only

Single crystal tube in torsion

001 cristallographic axis is in the direction of the tube axis

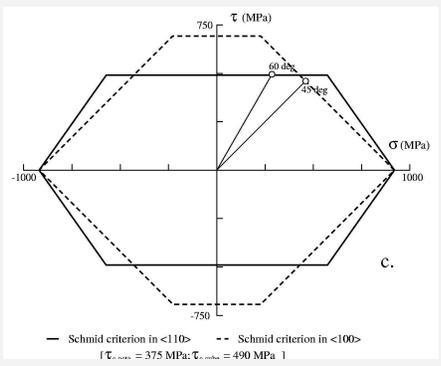
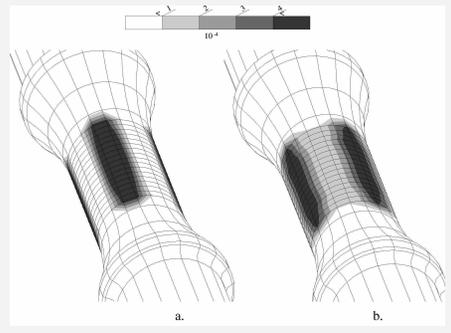


100 is a hard zone, 110 is a soft area

Strain jauges are in 100 and 001 areas

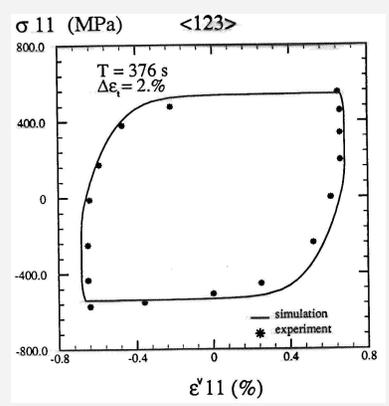
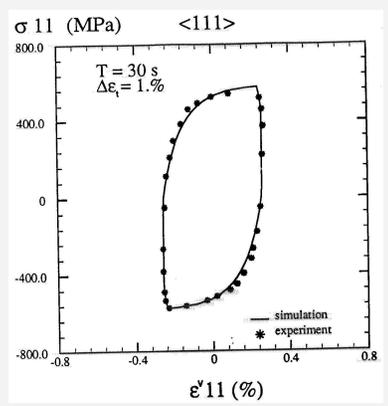
Experiments performed at ONERA

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



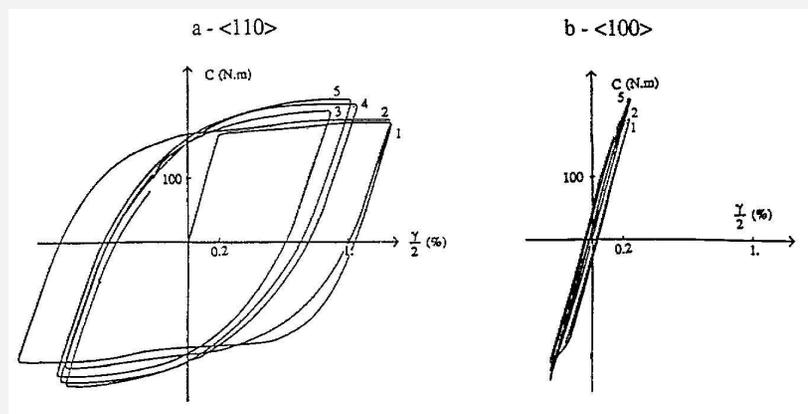
(more in [Nouailhas and Cailletaud, 1995])

Cyclic tests on AM1 superalloy



(more in [Méric et al., 1991, Hanriot et al., 1991])

Single crystal tube in torsion (2)



Strain jauges response in pure torsion

Equivalence between single crystal and von Mises

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

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

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

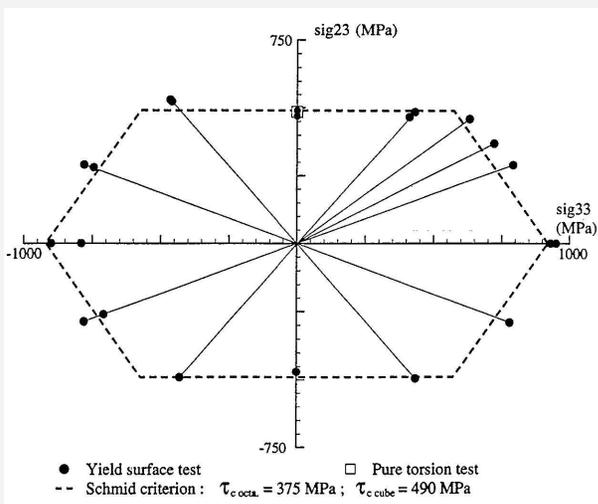
$$\dot{\epsilon}^P = \left\langle \frac{(\sigma - X) - R}{K} \right\rangle^n \text{ with } K = \frac{k}{m} \frac{1}{mM}^{1/n}, \quad X = \frac{x}{m}, \quad R = \frac{r}{m}$$

What is the best set of active slip systems ?

- Physical responses (Hill, Taylor)
- Algorithmic responses (many authors)

Are they consistent ?

Yield surface determined on the single crystal tube



Note that Hill's criterion give wrong results

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	$\frac{c}{Mm^2}$	$\frac{3c}{4}$	$\frac{2}{3c}$
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

Bishop and Hill

Find the stress state which...

- **Maximize** the the external power, written as

$$\mathcal{P}_e = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p$$

- The constraint is

$$g^s(\boldsymbol{\sigma}) = \tau_c^s - \boldsymbol{\sigma} : \mathbf{m}^s \geq 0$$

- The lagrangian function is then now:

$$\mathcal{F}_e(\boldsymbol{\sigma}, \dot{\mu}^s) = \mathcal{P}_e + \sum_s \dot{\mu}^s g^s$$

$$\frac{\partial \mathcal{F}_e}{\partial \boldsymbol{\sigma}} = \dot{\boldsymbol{\epsilon}}^p - \sum_s \mathbf{m}^s \dot{\mu}^s = 0 \quad \frac{\partial \mathcal{F}_e}{\partial \dot{\mu}^s} = \tau_c^s - \boldsymbol{\sigma} : \mathbf{m}^s = 0$$

- The multipliers $\dot{\mu}^s$ are nothing but plastic strain rates.

To find a stress tensor, find a set of plastic shear strain rates which are zero on the inactive slip systems, and positive on the active slip systems.

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Incremental form

Small strain, linear isotropic hardening

- (1) Strain partition:

$$\Delta \boldsymbol{\sigma} = \underline{\underline{\boldsymbol{\Lambda}}} : \left(\Delta \boldsymbol{\epsilon} - \sum_r \mathbf{m}^r \Delta p^r \right)$$

- (2) Criterion:

$$f^s = \tau^s - r^s = 0 \quad \text{with} \quad r^s = \sum_r h_{sr} p^r$$

$$\mathbf{m}^s : \Delta \boldsymbol{\sigma} - \sum_r h_{sr} \Delta p^r$$

Project (1) on \mathbf{m}^r to eliminate $\Delta \boldsymbol{\sigma}$, compute $\mathbf{m}^s : \Delta \boldsymbol{\sigma}$:

$$\sum_r \left(h_{rs} + \mathbf{m}^r : \underline{\underline{\boldsymbol{\Lambda}}} : \mathbf{m}^s \right) \Delta p^r = \mathbf{m}^s : \underline{\underline{\boldsymbol{\Lambda}}} : \Delta \boldsymbol{\epsilon}$$

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Taylor

Select a set of admissible shear rates $\dot{\gamma}^s$ for a prescribed plastic strain rate $\dot{\boldsymbol{\epsilon}}^p$ (assuming $\boldsymbol{\epsilon} \equiv \boldsymbol{\epsilon}^p$)

- **Minimize** the internal power of the material element:

$$\mathcal{P}_i = \sum_s \tau_c^s \dot{\gamma}^s$$

- The shear strain rates are submitted to the constraint:

$$\underline{\underline{\mathbf{g}}}(\dot{\boldsymbol{\epsilon}}^p) = \dot{\boldsymbol{\epsilon}}^p - \sum_s \mathbf{m}^s \dot{\gamma}^s = 0$$

- Let us define the lagrangian \mathcal{F}_i , and search for the saddle point

$$\mathcal{F}_i(\dot{\boldsymbol{\epsilon}}^p, \boldsymbol{\lambda}) = \mathcal{P}_i + \boldsymbol{\lambda} : \underline{\underline{\mathbf{g}}}$$

$$\frac{\partial \mathcal{F}_i}{\partial \boldsymbol{\lambda}} = \dot{\boldsymbol{\epsilon}}^p - \sum_s \mathbf{m}^s \dot{\gamma}^s = 0 \quad \frac{\partial \mathcal{F}_i}{\partial \dot{\gamma}^s} = \tau_c^s - \boldsymbol{\lambda} : \mathbf{m}^s = 0$$

- The tensor $\boldsymbol{\lambda}$ is nothing but the stress tensor.

To find the set of shear strain rates, which minimizes internal power, find a stress tensor which obeys the yield conditions, i.e. allows to built resolved shear stresses which reach τ_c^s on the active slip systems and which are smaller than τ_c^s on the inactive ones.

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Synthesis of the various conditions

- Taylor, Bishop–Hill

$$\boldsymbol{\sigma}^* : \dot{\boldsymbol{\epsilon}}^p \leq \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p = \sum_s \tau_c^s \dot{\gamma}^s \leq \sum_s \tau_c^s \dot{\gamma}^s$$

- In the thermodynamical approach, the dissipation can be written:

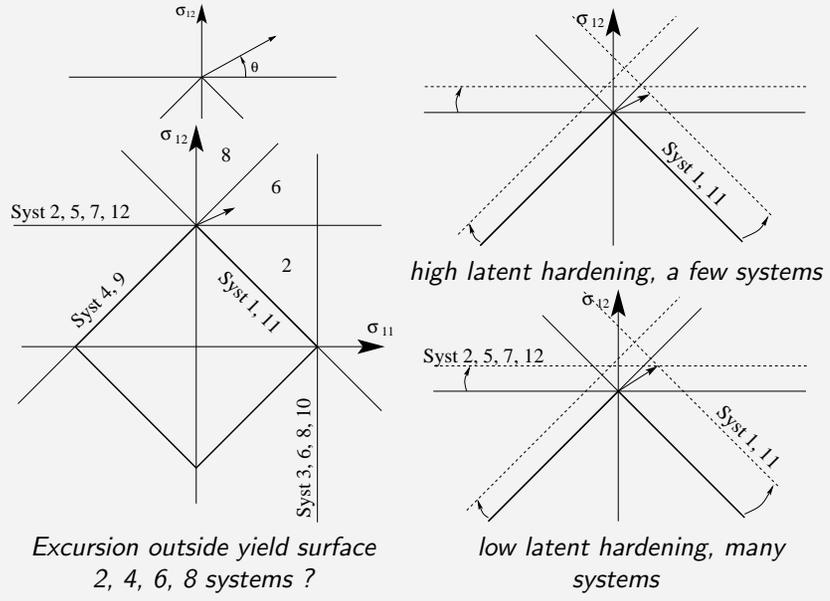
$$\Phi_1 = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p - \sum_s r^s \dot{\gamma}^s$$

- The variables r^s are the increase of critical resolved shear stress. One has

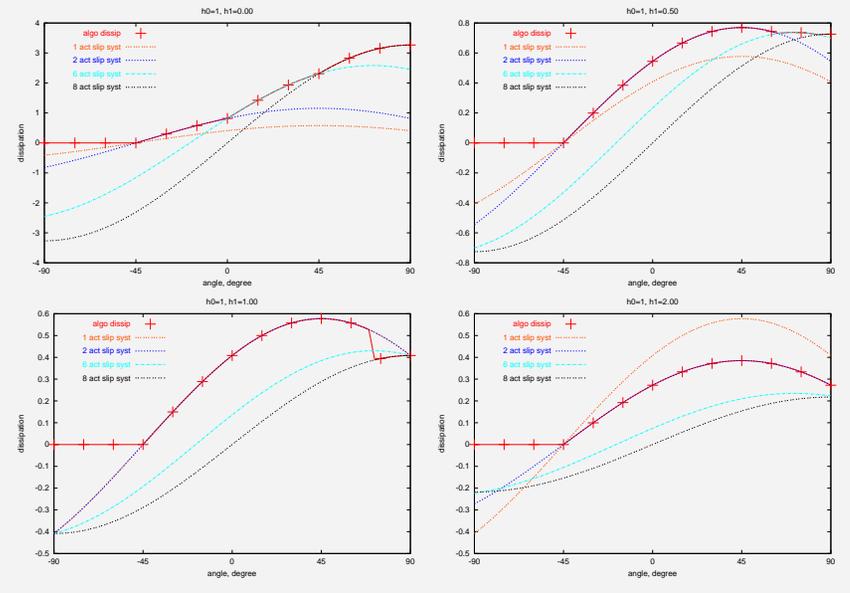
$$\Phi_1 = \sum_s r_0^s \dot{\gamma}^s$$

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Application to a specific loading just outside yield surface



Evaluation of the dissipation for various values of latent hardening



Algorithmic form

Internal variables ϵ^e et p^s ($s = 1 \dots N$)

- (1) Strain partition:

$$\mathcal{F}_e = -\Delta \epsilon^* + \Delta \epsilon^e + \sum_r \mathbf{m}^r \Delta p^r$$

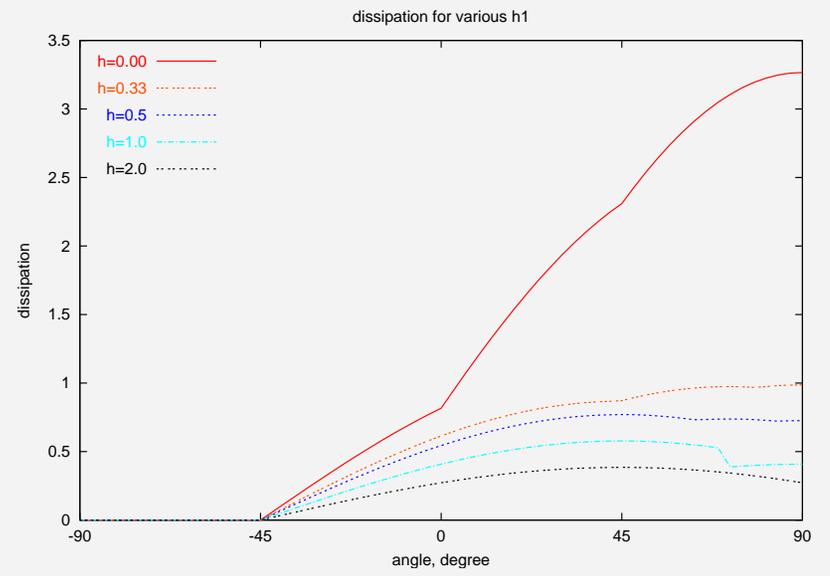
- (2) Criterion for a plastic model:

$$\mathcal{F}_p^s = \left| \mathbf{m}^s : \underline{\underline{\Lambda}} : (\epsilon^e + \Delta \epsilon^e) \right| - \tau_0 - \sum_r h_{sr} (p^r + \Delta p^r)$$

- (2bis) Viscoplastic model:

$$\mathcal{F}_p^s = \left| \mathbf{m}^s : \underline{\underline{\Lambda}} : (\epsilon^e + \Delta \epsilon^e) \right| - \tau_0 - \sum_r h_{sr} (p^r + \Delta p^r) - K \left(\frac{\Delta p^s}{\Delta t} \right)^{1/n}$$

Evaluation of the dissipation for various values of latent hardening



Evaluation of the dissipation for various values of latent hardening

- 1 active system:

$$D = \frac{\sqrt{6}(\cos \theta + \sin \theta)}{6h_0}$$

- 2 active systems:

$$D = \frac{\sqrt{6}(\cos \theta + \sin \theta)}{3(h_0 + h_1)}$$

- 6 active systems:

$$D = \frac{\sqrt{6}(\cos \theta + 3 \sin \theta)}{3(h_0 + 5h_1)}$$

- 8 active systems:

$$D = \frac{4\sqrt{6} \sin \theta}{3(h_0 + 7h_1)}$$

Number of active slip systems according to h_1 values

h_1	0-2	2-6	6-8
0	-45	0	45
0.33	-45	45	80
0.50	-45	66	84
1.	-45	87	90
1.5	-45	88	90
2.	-45	90	90

The algorithmic solution is not always in good agreement with the maximum dissipation principle

A generic formulation of single crystal models

$$\tau^\alpha = B^\alpha \pm S^\alpha \pm \hat{f}_v(\dot{\gamma}^\alpha, R^\alpha)$$

- Kinematic hardening, B^α (back stress)
- Additive isotropic hardening, S^α , (friction stress)
- Multiplicative isotropic hardening, R^α , (drag stress)

One can find associated state variables, resp. $b^\alpha, s^\alpha, r^\alpha$

What is the best set of active slip systems (2) ?

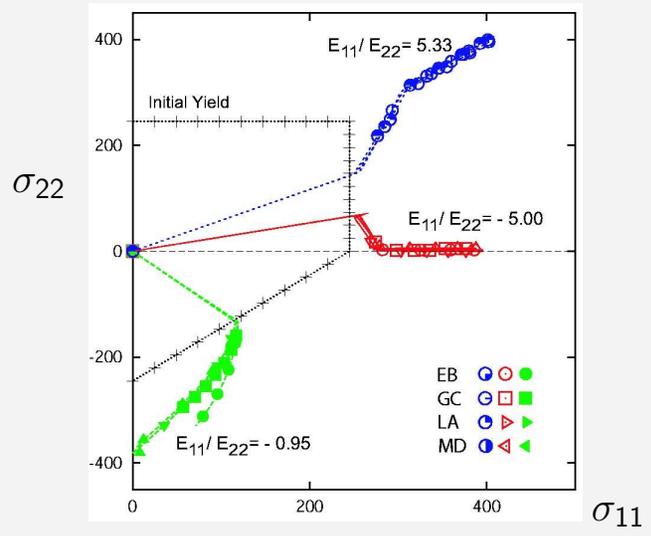
- Tests responses on critical loading paths
- Various subroutines tested: Anand (LA), Busso (EB), Cailletaud (GC)(code Zebulon), McDowell (MD)

(more in [Busso and Cailletaud, 2005])

Functions for the different single crystal models

Model	Equation
$\dot{S}_{GC}^\alpha =$	$\sum_\beta h^{\alpha\beta} [h_s - d_s s^\beta] \dot{\gamma}^\beta $
$\dot{S}_{EB}^\alpha =$	$\sum_\beta h^{\alpha\beta} (h_s - d_s [S^\beta - S_0]) \dot{\gamma}^\beta $
$\dot{R}_{LA}^\alpha =$	$\sum_\beta h_s [q_l + (1 - q_l) \delta^{\alpha\beta}] \left\{ 1 - \frac{R^\beta}{R^*} \right\}^a \dot{\gamma}^\beta $
$\dot{R}_{DM}^\alpha =$	$\sum_\beta q_l h_s \dot{\gamma}^\beta - (q_l - 1) h_s \dot{\gamma}^\alpha - d_s R^\alpha \left[\sum_\beta q_l \dot{\gamma}^\beta - (q_l - 1) \dot{\gamma}^\alpha \right]$
$\dot{B}^\alpha =$	$[h_B \text{sign}(\dot{\gamma}^\alpha) - d_B B^\alpha] \dot{\gamma}^\alpha $

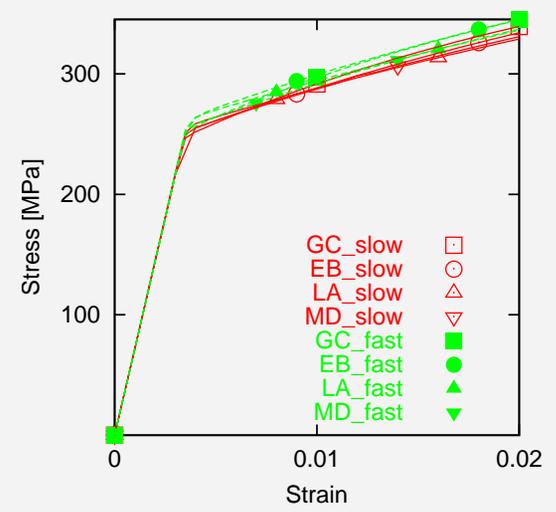
Loading paths in the 11-22 plane



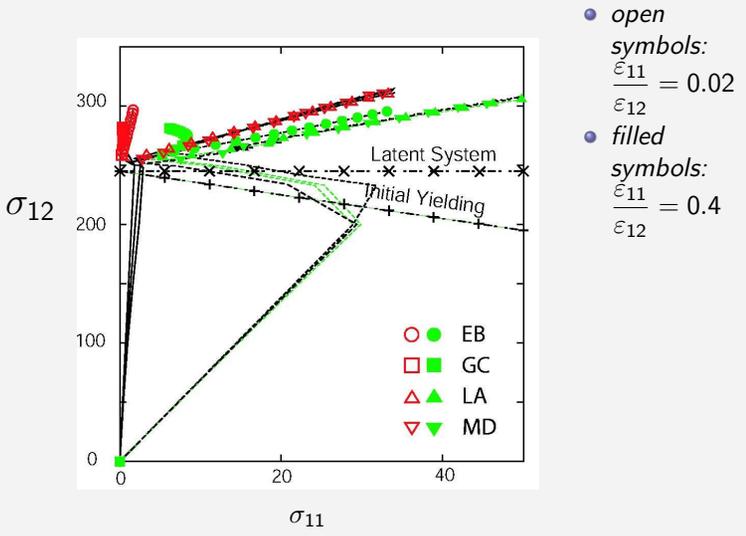
Functions for the different single crystal models

Function	GC	EB	LA	DM
f^α	$ \tau^\alpha - B^\alpha - S^\alpha - S_0$	$ \tau^\alpha - B^\alpha - S^\alpha$	$ \tau^\alpha - B^\alpha $	$ \tau^\alpha - B^\alpha $
$ \dot{\gamma}^\alpha $	$\dot{\gamma}_0 \left\langle \frac{f^\alpha}{\tau_0} \right\rangle^n$	$\dot{\gamma}_0 \exp \left\{ -\frac{F_0}{k\theta} \left\langle 1 - \left\langle \frac{f^\alpha}{\tau_0} \right\rangle^p \right\rangle^q \right\}$	$\dot{\gamma}_0 \left\langle \frac{f^\alpha}{R^\alpha} \right\rangle^n$	$\dot{\gamma}_0 \left\langle \frac{f^\alpha}{R^\alpha} \right\rangle^n$
$\hat{r}_r^\alpha \{r^\alpha\}$	-	-	$\frac{1}{2} h_s \sum_\alpha (r^\alpha)^2$	$\frac{1}{2} h_s \sum_\alpha (r^\alpha)^2$
$\hat{r}_s^\alpha \{s^\alpha\}$	$\frac{1}{2} h_s \sum_\alpha (s^\alpha)^2$	$\frac{1}{2} h_s \sum_\alpha (s^\alpha)^2$	-	-
$\hat{r}_b^\alpha \{b^\alpha\}$	$\frac{1}{2} h_b \sum_\alpha (b^\alpha)^2$	$\frac{1}{2} h_b \sum_\alpha (b^\alpha)^2$	$\frac{1}{2} h_b \sum_\alpha (b^\alpha)^2$	$\frac{1}{2} h_b \sum_\alpha (b^\alpha)^2$
R^α	-	-	$h_s r^\alpha$	$h_s r^\alpha$
S^α	$\sum_\beta h^{\alpha\beta} s^\beta$	$h_s s^\alpha$	-	-
B^α	$h_b b^\alpha$	$h_b b^\alpha$	$h_b b^\alpha$	$h_b b^\alpha$

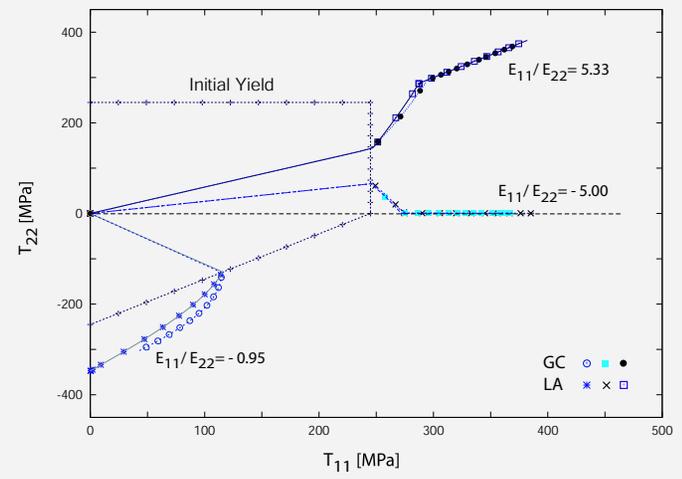
Identification of the four models for pure tension



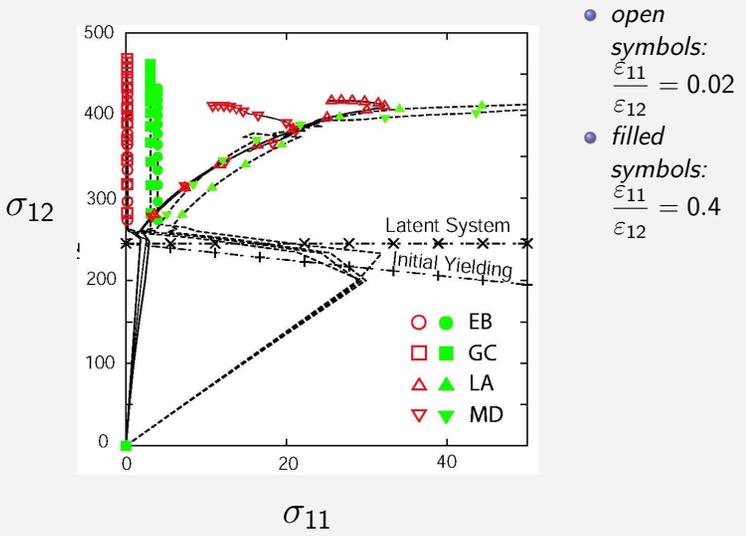
Loading paths in the 11-12 plane, self-hardening only



Loading paths in the 11-22 plane



Loading paths in the 11-12 plane, Taylor type hardening

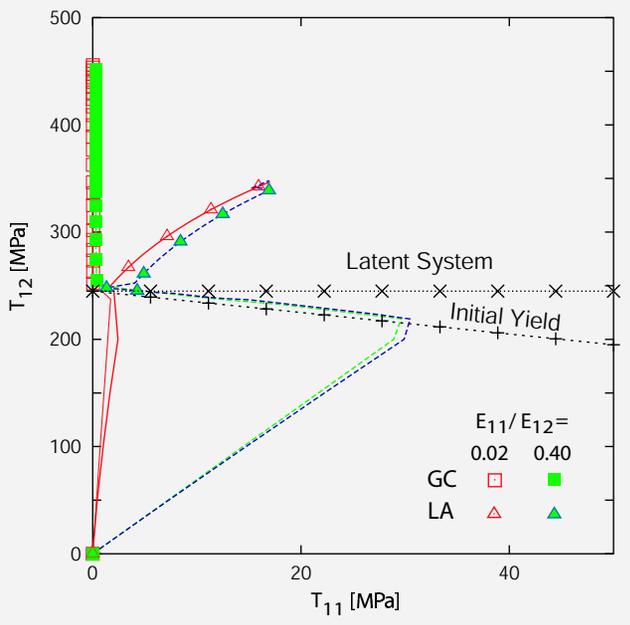


Algorithmic solution to select the slip systems

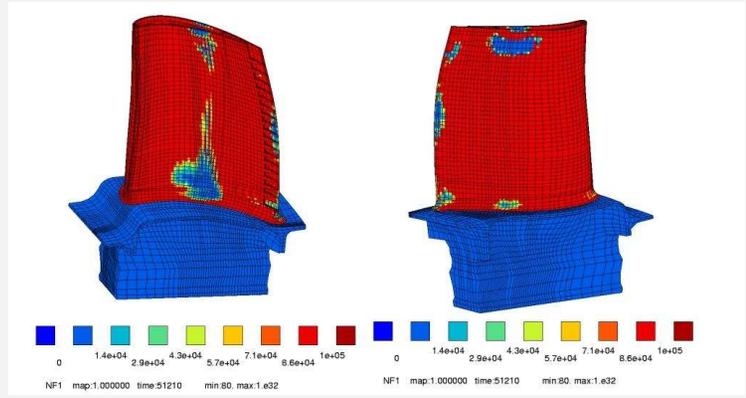
Plastic models

- Loop on the slip systems, select the slip systems for which $f_s > 0$, check that Δp^r is positive, eliminate r such as $\Delta p^r < 0$ (Simo, Miehe, Zebulon)
- SDV decomposition (Anand)

Loading paths in the 11-12 plane

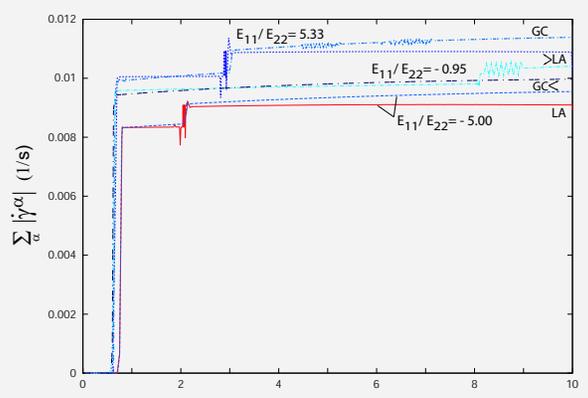


Numerical simulations of single crystal turbine blades (Snecma)



Thermal + mechanical loading
Post treatment needed for life prediction

History of the total strain rate for 11-22 loadings



A model using dislocations

$$\dot{\gamma}^s = \dot{\gamma}_0 \left(\frac{\tau^s}{\tau_\mu^s} \right)^{1/m}$$

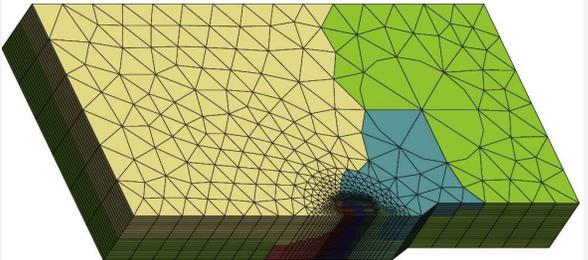
$$\tau_\mu^s = \alpha \mu b \left(\sum_{r=1}^N h_{sr} \rho^r \right)^{1/2}$$

$$\dot{\rho}^s = \frac{1}{b} \left(\frac{\left(\sum_{r=1}^N a^{sr} \rho^r \right)^{1/2}}{K} - 2y_c \rho^s \right) \dot{\gamma}^s$$

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

Crack in single crystals: discussion about plastic zones

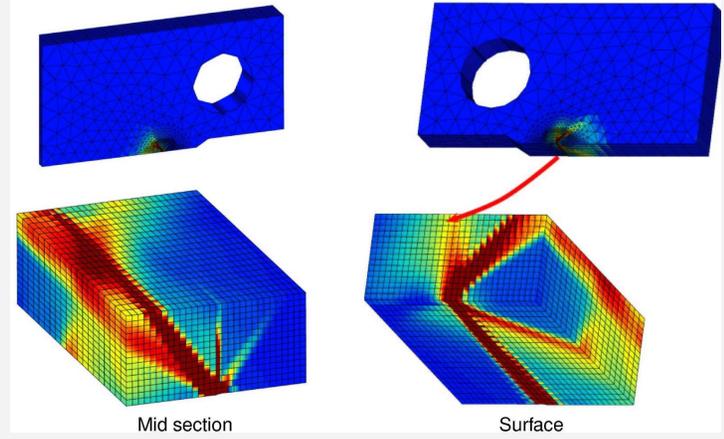
Simulation of CT specimens with various orientations



Flouriot PhD, 2000

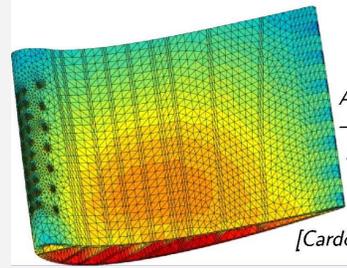
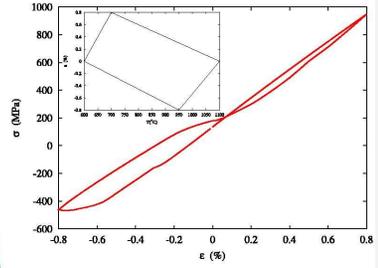
Crack in single crystals: 3D effects

Rice solution on the symmetry plane



Homogenization of multiperforated single crystals

- Traction-LCF
- Torsion
- Essai anisotherme
- Structure



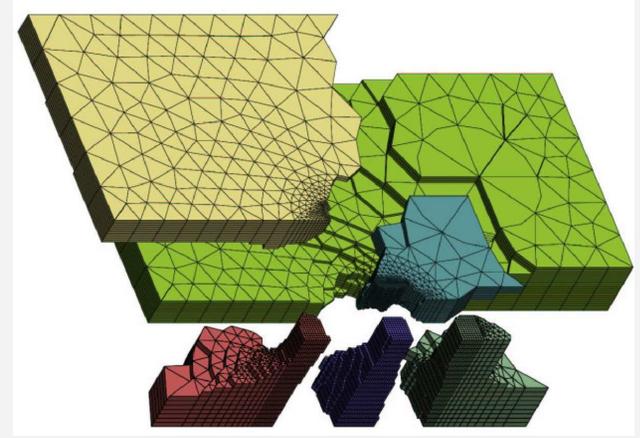
Aube de turbine
→ Superalliage monocristallin
à base de nickel

[Cardona, 2000]

Development of a model to account for hole distribution
Cardona PhD, 2000

Crack in single crystals: mesh of a CT specimen

Mesh with domain decomposition, ready for parallel computing

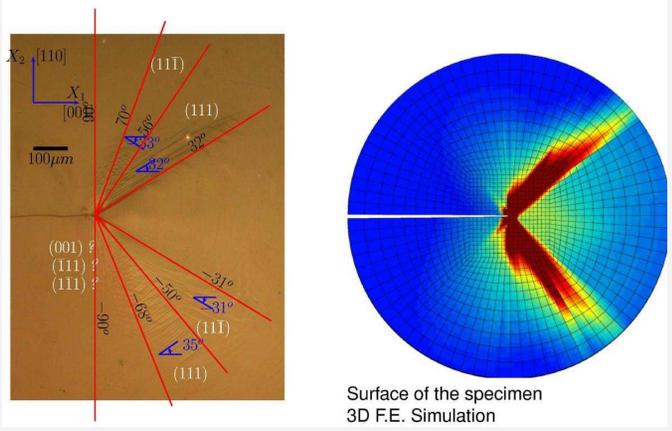


Literature

- **Books**
[Havner, 1992, Teodosiu, 1997]
- **Models, isotropic hardening, plastic or viscoplastic**
[Taylor, 1938, Bishop and Hill, 1951, Koiter, 1960, Mandel, 1965, Mandel, 1971, Hill, 1966, Hill and Rice, 1972, Kocks and Brown, 1966, Chin and Mammel, 1969, Kocks, 1970, Rice, 1970, Rice, 1971, Asaro and Rice, 1977, Franciosi et al., 1980, Asaro, 1983b, Asaro, 1983a, Franciosi, 1985, Tabourot et al., 1997]
- **New generation of models, appropriate for complex/cyclic loadings**
[Méric et al., 1991, Hanriot et al., 1991, Jordan and Walker, 1985, Méric et al., 1994, Nouailhas and Cailletaud, 1995, Busso and McClintock, 1996, Forest et al., 1996, Nouailhas and Cailletaud, 1996, Busso and Cailletaud, 2005]
- **Numerical integration**
[Pierce et al., 1985, Asaro and Needleman, 1985, Méric and Cailletaud, 1991, Cuitino and Ortiz, 1992, Simo and Hughes, 1997, Schröder and Miehe, 1997, Anand and Kothari, 1996, McGinty, 2001]
- **Cracks**
[Flourirot et al., 2003]
- **Industrial applications**
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Crack in single crystals: comparison with experiments

Elastic and plastic zones



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