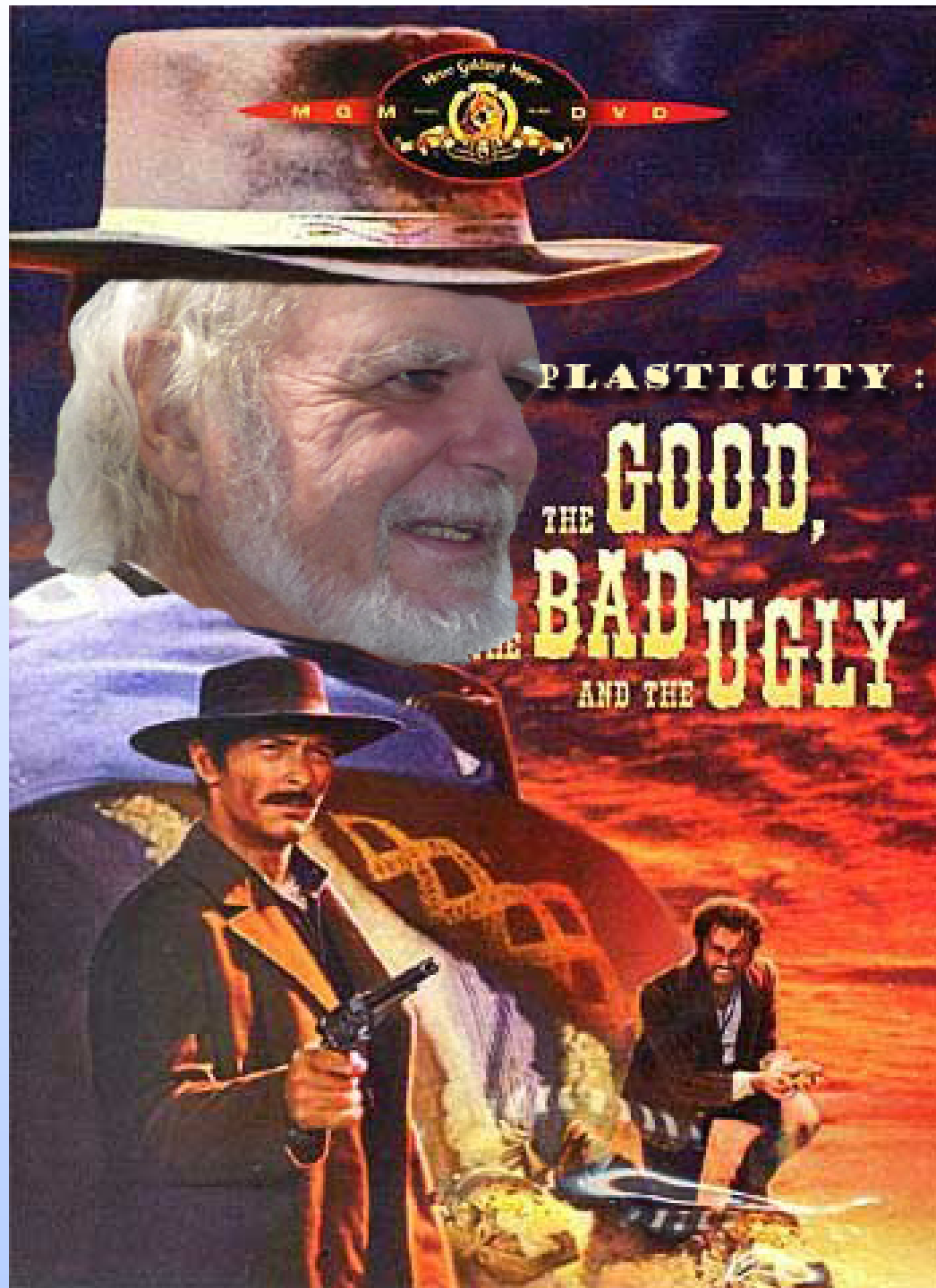


Plasticity :
the Good,
the Bad
and the Ugly

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1. How does plasticity manifest itself?

Macroscopic scale

Plasticity : *πλασσειν* : To mold (or give a shape)*.



Part of the deformation is not recovered upon unloading

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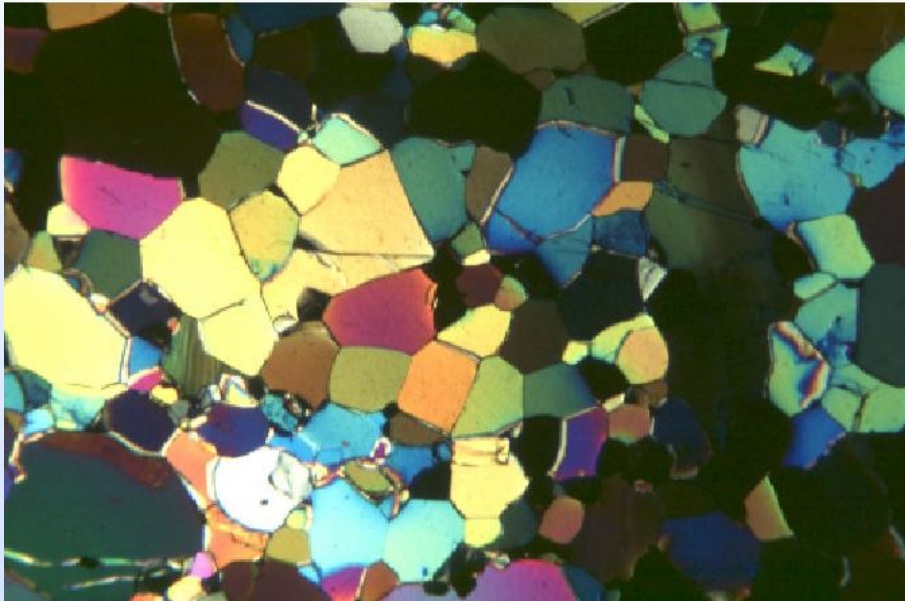
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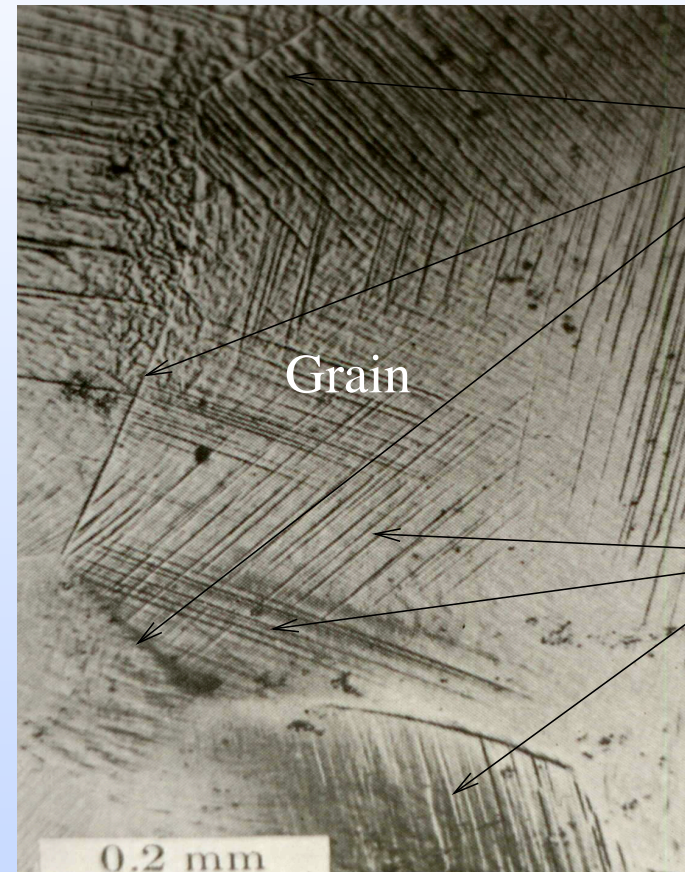
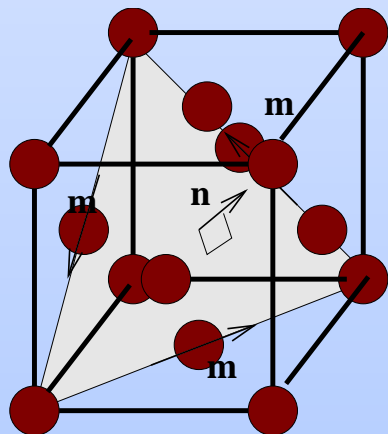
Irreversible deformation is accompanied by energy dissipation..

*By extension "Brain plasticity : ability of the brain to (re)model itself.

Mesoscopic scale (for polycrystalline solids)



Grains with different orientations but identical crystalline structure.

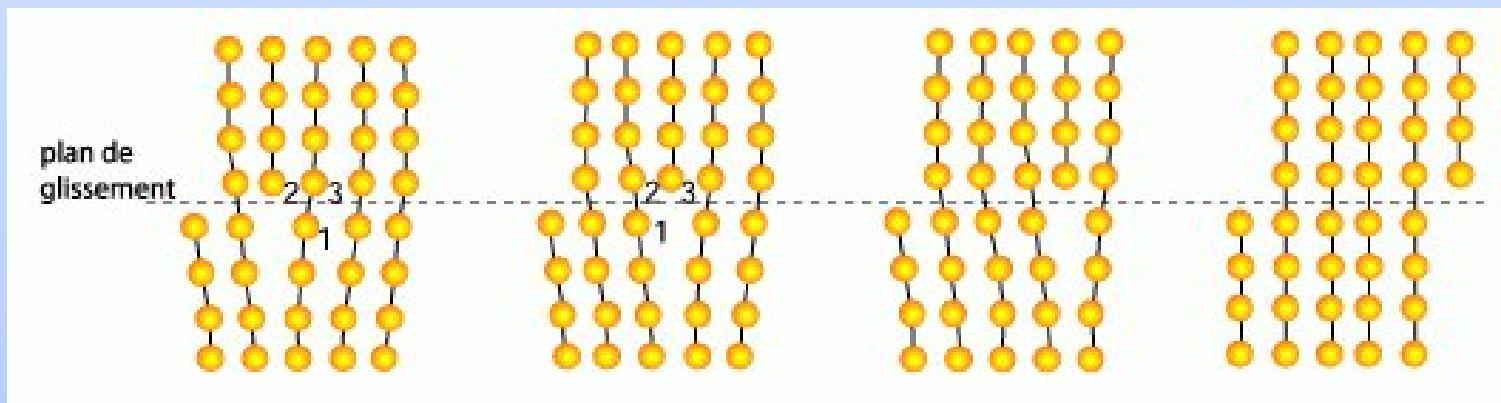
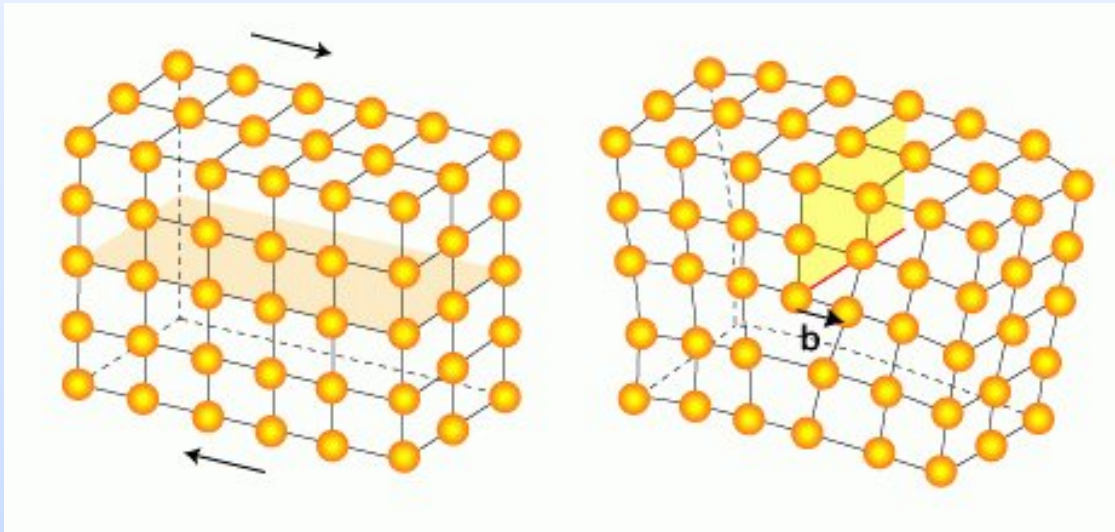


Deformation by slip along preferred directions.

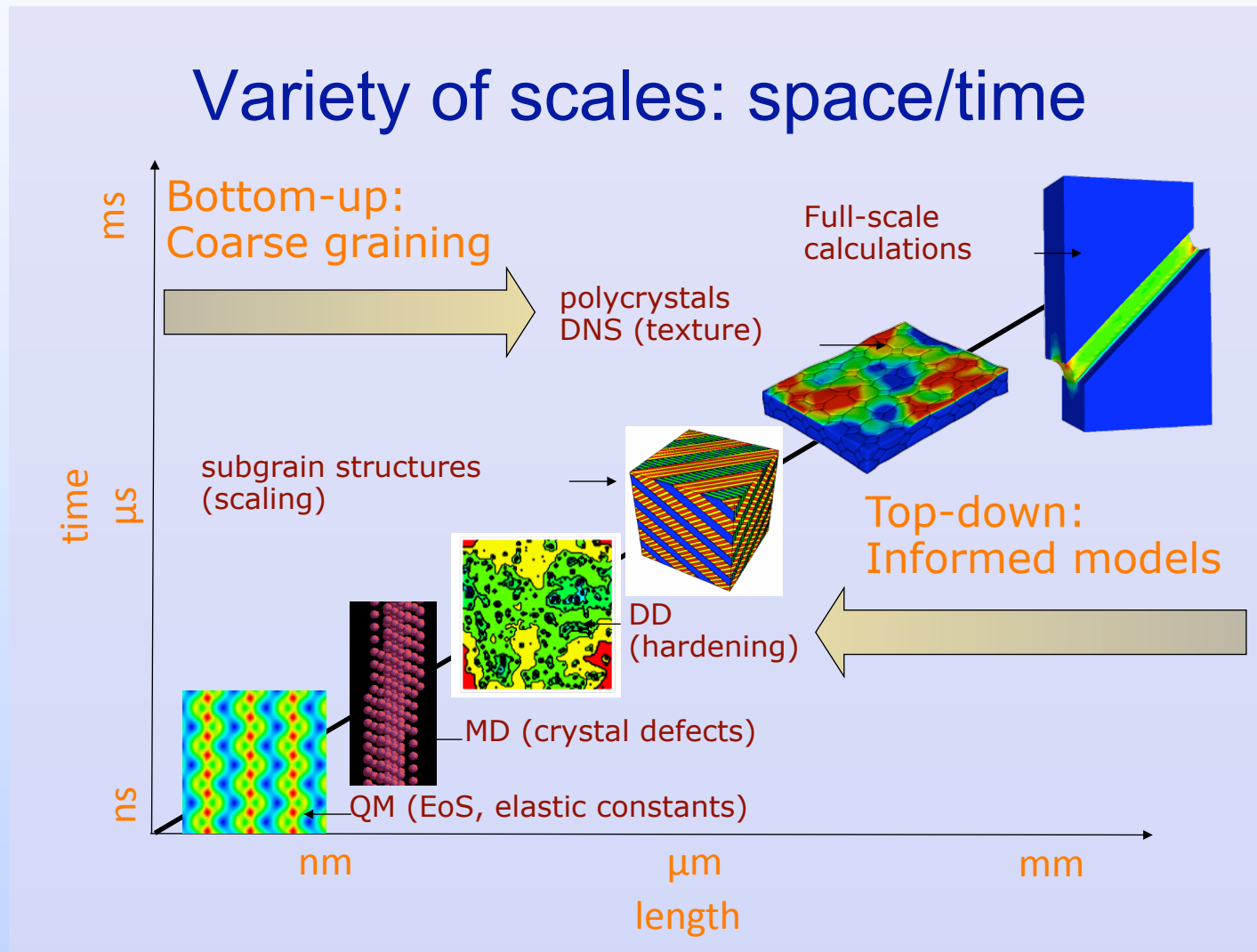
Deformation is highly localized and heterogeneous.

Microscopic scale

Plastic slip is due to the creation of defects (**dislocations**) and to their motion along preferred directions in a crystalline lattice. **Typical density** $10^{14}/\text{mm}^2$. **Bursts of dislocations** : **"intermittency"** of plastic deformation.



Plasticity : a cascade of scales



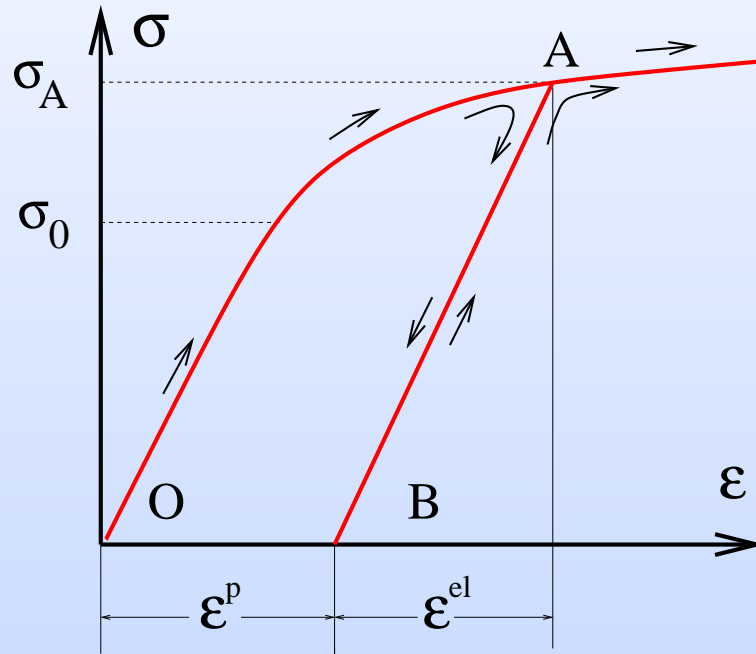
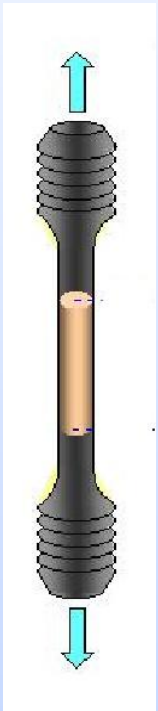
- Russian dolls : at least 6 decades in space!
- Small scale models : provide information to macroscopic models.
- Spatial scale \Rightarrow time scale.

Aim of this talk :

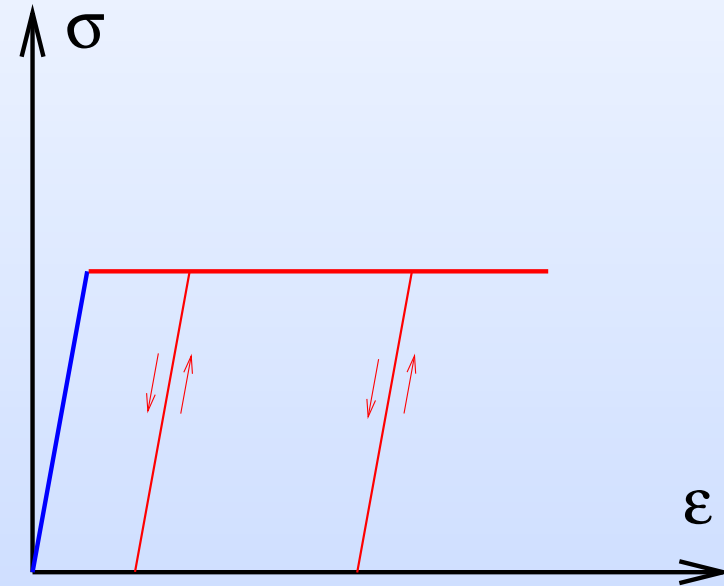
- Discuss **mathematical models** currently used to describe Plasticity and their capacity to account for specific features of the plastic deformation :
 - **Localization.**
 - **Intermittency.**
- Discuss how these features are affected by **upscaling** (homogenization.

2. Mathematics of Plasticity

Seen from a macroscopic perspective



Plasticity with hardening



Perfect (ideal) Plasticity

1d model : $\varepsilon = \varepsilon^e + \varepsilon^p$, $\varepsilon^e = \frac{\sigma}{E}$, $|\sigma| \leq \sigma_0$, $\dot{\varepsilon}^p = \dot{\lambda} \frac{\sigma}{|\sigma|}$, $\dot{\lambda} \geq 0$, $= 0$ when $|\sigma| < \sigma_0$,

Plastic dissipation : $d(\dot{\varepsilon}^p) = \sigma_0 |\dot{\varepsilon}^p|$.

Three-dimensional formulation of macroscopic Plasticity

Strain decomposition :

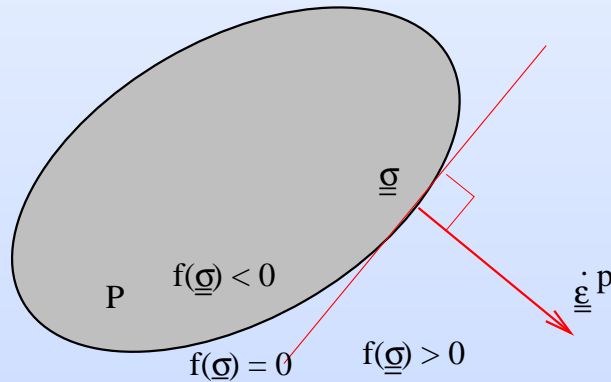
$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p, \quad \boldsymbol{\varepsilon}^e = \mathbf{M} : \boldsymbol{\sigma},$$

Stresses are physically limited :

P Plasticity domain : closed convex in $\mathbb{R}_s^{3 \times 3}$,

$$\boldsymbol{\sigma} \in P,$$

Flow rule :



$$\dot{\boldsymbol{\varepsilon}}^p \in \partial I_P(\boldsymbol{\sigma}).$$

Free-energy and plastic dissipation :

$$w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) : \mathbf{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p), \quad d(\dot{\boldsymbol{\varepsilon}}^p) = \text{Sup}_{\boldsymbol{\tau} \in P} \boldsymbol{\tau} : \dot{\boldsymbol{\varepsilon}}^p.$$

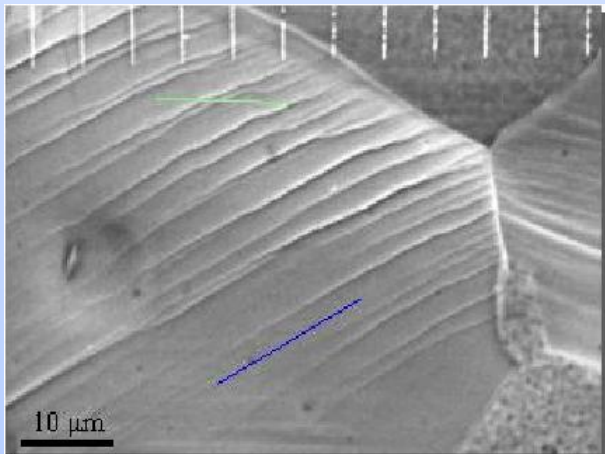
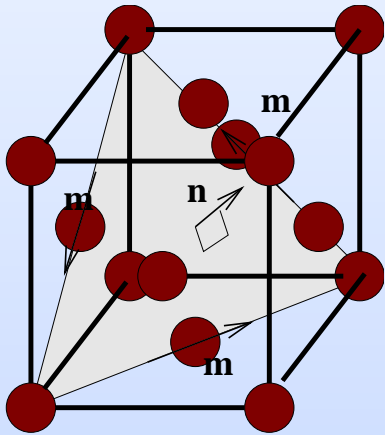
Note that d is positively homogeneous of degree one : $d(\lambda \dot{\boldsymbol{\varepsilon}}^p) = \lambda d(\dot{\boldsymbol{\varepsilon}}^p)$, $\lambda \geq 0$.

Ex : von Mises Plasticity : $P = \{\boldsymbol{\sigma} : \sigma_{\text{eq}} \leq \sigma_0\}$, $d(\dot{\boldsymbol{\varepsilon}}^p) = \sigma_0 \dot{\boldsymbol{\varepsilon}}_{\text{eq}}^p$.

Crystal Plasticity : single crystal

Slip only in specific planes $\mathbf{n}^{(k)}$, along specific directions $\mathbf{m}^{(k)}$.

N slip systems $(\mathbf{n}^{(k)}, \mathbf{m}^{(k)})$.



Resolved shear on the k -th slip system :

$$\tau^{(k)} = (\boldsymbol{\sigma} \cdot \mathbf{n}^{(k)}) \cdot \mathbf{m}^{(k)} = \boldsymbol{\sigma} : \mathbf{m}^{(k)} \otimes_s \mathbf{n}^{(k)}.$$

$$\begin{aligned} \text{Sup}_{k=1, \dots, N} \tau^{(k)} &\leq \tau_c \\ \dot{\boldsymbol{\epsilon}}^p &= \sum_{k=1}^N \dot{\gamma}^{(k)} \mathbf{m}^{(k)} \otimes_s \mathbf{n}^{(k)} \end{aligned}$$

Same form as macroscopic Plasticity :

$$P = \{ \boldsymbol{\sigma} \text{ such that } f^{(k)}(\boldsymbol{\sigma}) \leq 0, k = 1, \dots, N \}$$

$$f^{(k)}(\boldsymbol{\sigma}) = \boldsymbol{\sigma} : \mathbf{m}^{(k)} \otimes_s \mathbf{n}^{(k)} - \tau_c,$$

$$\dot{\boldsymbol{\epsilon}}^p = \sum_{k=1}^N \dot{\gamma}^{(k)} \frac{\partial f^{(k)}}{\partial \boldsymbol{\sigma}}(\boldsymbol{\sigma}),$$

$$\boldsymbol{\sigma} \in P, \quad \dot{\boldsymbol{\epsilon}}^p \in \partial I_P(\boldsymbol{\sigma}).$$

Boundary Value Problem (BVP) for a perfectly plastic body

Compatibility (small strains) :

$$\boldsymbol{\varepsilon} = \frac{1}{2} (\nabla \mathbf{u} + {}^T \nabla \mathbf{u}),$$

Equilibrium :

$$\operatorname{div}(\boldsymbol{\sigma}) + \mathbf{F} = 0,$$

Constitutive relations :

$$\begin{aligned} \boldsymbol{\varepsilon} &= \mathbf{M} : \boldsymbol{\sigma} + \boldsymbol{\varepsilon}^p, \\ \boldsymbol{\sigma} &\in P, \quad \dot{\boldsymbol{\varepsilon}}^p \in \partial I_P(\boldsymbol{\sigma}) \end{aligned}$$

Boundary conditions :

$$\mathbf{T} = \boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{T}^d \quad \text{on } S_T, \quad \mathbf{u} = \mathbf{u}^d \quad \text{on } S_u.$$

Loading history :

$$\mathbf{F}(\mathbf{x}, t), \mathbf{T}^d(\mathbf{x}, t), \mathbf{u}^d(\mathbf{x}, t)$$

Existence and uniqueness of a displacement field $\mathbf{u}(\mathbf{x}, t)$ and of a stress field $\boldsymbol{\sigma}(\mathbf{x}, t)$ solving BVP ?

Stress field : the Good !

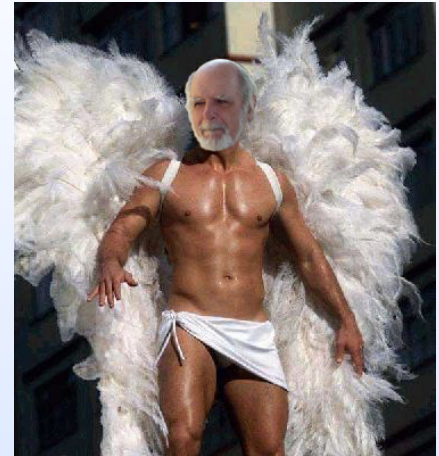
A necessary condition for a solution σ is that there exists at least one statically and plastically admissible field.

statically admissible : $\sigma \in \mathcal{S}(t)$

$$\mathcal{S}(t) = \left\{ \sigma^*, \operatorname{div}(\sigma^*) + \mathbf{F} = \mathbf{0} \text{ in } \Omega, \sigma^* \cdot \mathbf{n} = \mathbf{T}^d \text{ on } S_T \right\}.$$

plastically admissible : $\sigma \in \mathcal{P}$

$$\mathcal{P} = \left\{ \sigma^*, \text{ such that } \sigma^*(\mathbf{x}) \in P(\mathbf{x}) \quad \forall \mathbf{x} \in \Omega. \right\}$$



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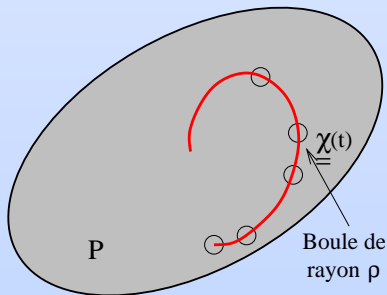


Safe load condition

Assume that there exists a stress field $\chi(\mathbf{x}, t)$ such that :

1) $\chi(\mathbf{x}, t) \in \mathcal{S}(t) \cap \mathcal{P},$

2) $\exists \rho > 0, \text{ such that } \chi(\mathbf{x}, t) + \boldsymbol{\tau} \in \mathcal{P} \quad \forall \boldsymbol{\tau} \in \mathbb{R}_s^{3 \otimes 3}, \|\boldsymbol{\tau}\| \leq \rho,$



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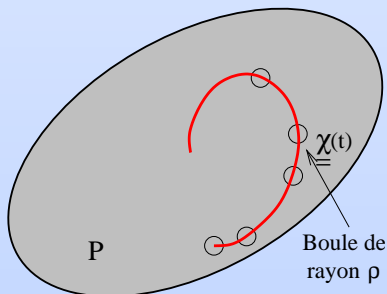


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Then, under classical assumptions (ensuring the existence of a solution in elasticity) + the safe load condition, there exists a unique stress field $\sigma(\mathbf{x}, t)$ solution of the problem (Moreau, 70's) :

$$\sigma \in W^{1,2}(0, T, L^2(\Omega)^9).$$

Displacement field : the Bad !



Displacement field : the Bad !



Elastic energy and plastic dissipation must remain finite :

$$\int_{\Omega} w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) d\mathbf{x} < +\infty, \quad w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) : \mathbf{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p), \quad \int_{\Omega} d(\dot{\boldsymbol{\varepsilon}}^p) d\mathbf{x} < +\infty.$$

d positively homogeneous of degree 1 d grows like $\|\dot{\boldsymbol{\varepsilon}}^p\|$,

$$\int_{\Omega} d(\dot{\boldsymbol{\varepsilon}}^p) d\mathbf{x} < +\infty \quad \Leftrightarrow \quad \dot{\boldsymbol{\varepsilon}}^p \in M^1(\Omega) = \text{bounded measures,}$$

Bounded measures are worse than L^1 functions (think of a Dirac mass) !

$$\int_{\Omega} w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p) d\mathbf{x} < +\infty \quad \Leftrightarrow \quad \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p \in L^2(\Omega),$$

$\boldsymbol{\varepsilon}$ and $\boldsymbol{\varepsilon}^p$ are both likely to be bounded measures :

$$BD(\Omega) = \left\{ \mathbf{v} \in L^1(\Omega)^N, \quad \varepsilon_{ij}(\mathbf{v}) \text{ is a bounded measure} \right\}.$$

Under the safe load assumption, solutions (velocity field) do exist in $BD(\Omega)$ (PS 78).

$$\mathbf{u} \in L_w^2(0, T; BD(\Omega))$$

- **Weak** solutions, obtained as limits of viscous problems.

Under the safe load assumption, solutions (velocity field) do exist in $BD(\Omega)$ (PS 78).

$$\dot{\mathbf{u}} \in L_w^2(0, T; BD(\Omega))$$

- **Weak** solutions, obtained as limits of viscous problems.
- **Non-smooth solutions. No Korn's inequality in $BV(\Omega)^N$:**

$$BD(\Omega) \neq BV(\Omega)^N.$$

- **Trace theorems hold :**

$$\forall \mathbf{u} \in BD(\Omega), \quad \forall S \subset \Omega, \exists \mathbf{u}^+, \mathbf{u}^- \text{ traces of } \mathbf{u} \text{ on } S, \\ \boldsymbol{\varepsilon} = (\mathbf{u}^+ - \mathbf{u}^-) \otimes_s \mathbf{n} \delta_S.$$

- Plastic dissipation not only in the bulk but also on surfaces (slip lines) : For elements of $BD(\Omega)$ for which $\boldsymbol{\varepsilon}(\mathbf{u})$ has a regular part on $\Omega - S$ and a Dirac part on S

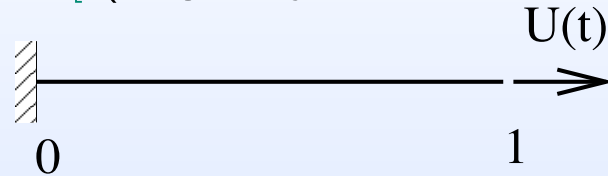
$$\boldsymbol{\varepsilon}(\mathbf{u}) = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p, \quad \boldsymbol{\varepsilon}^e \in L^2(\Omega), \quad \boldsymbol{\varepsilon}^p \in M^1(\Omega),$$



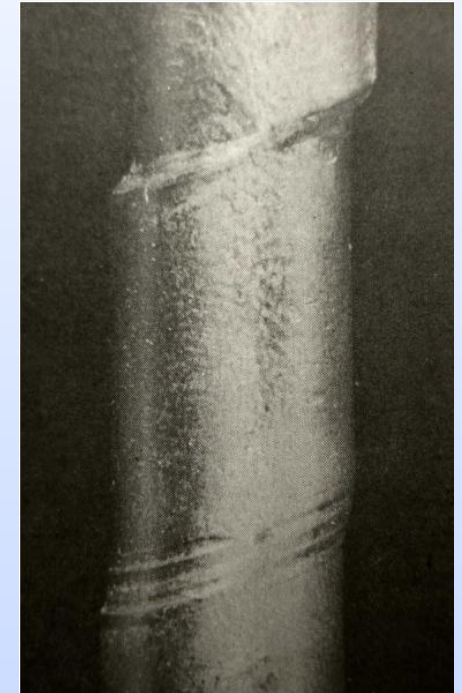
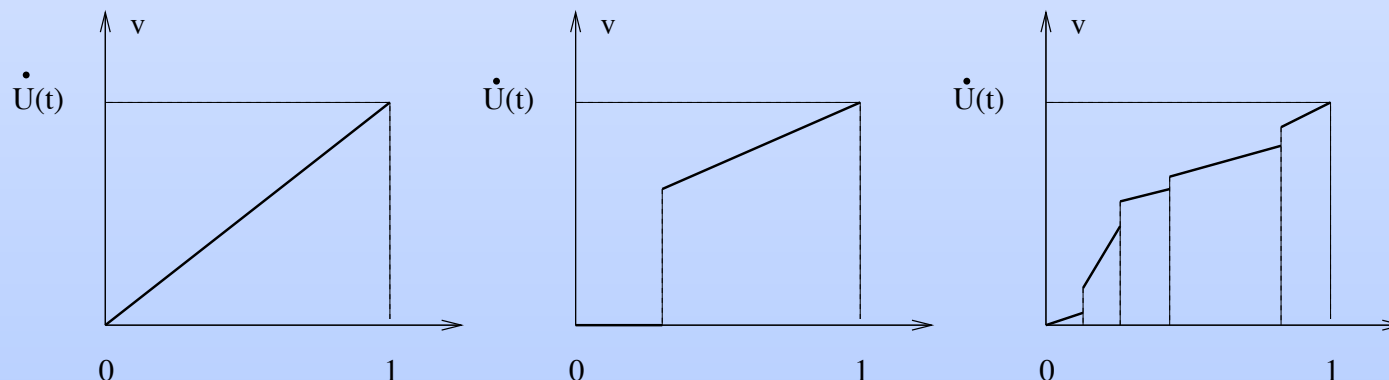
$$\text{Dissipation} = \int_{\Omega - S} d(\dot{\boldsymbol{\varepsilon}}^p) \, d\mathbf{x} + \int_S d((\dot{\mathbf{u}}^+ - \dot{\mathbf{u}}^-) \otimes_s \mathbf{n}) \, dS$$

Non-uniqueness and non-smoothness of solutions : the Ugly !

A 1d-example $\Omega =]0, 1[$ (single crystal with 1 slip system)



- $P = \{\sigma, |\sigma| \leq \sigma_0\}$, loading : $f = 0$, $u(0) = 0$, $u(1) = U(t) \geq 0$
- Safe-load condition : satisfied with $\chi = 0$. No limit-load !
- Elastic solution $u(x, t) = U(t)x$, $\sigma(t) = EU(t)$.
- First plastification when $t = t_1$, $U(t_1) = \sigma_0/E$. When $t \geq t_1$, $\sigma = \sigma_0$ (full plastification, but no limit on $U(t)$), **any non decreasing function $v \in BV(]0, 1[)$ such that $v^+(1) = \dot{U}(t)$ is a solution for the velocity field.**



Uniaxial tension single crystal (Zinc).

Infinitely many continuous solutions, infinitely many discontinuous solutions !

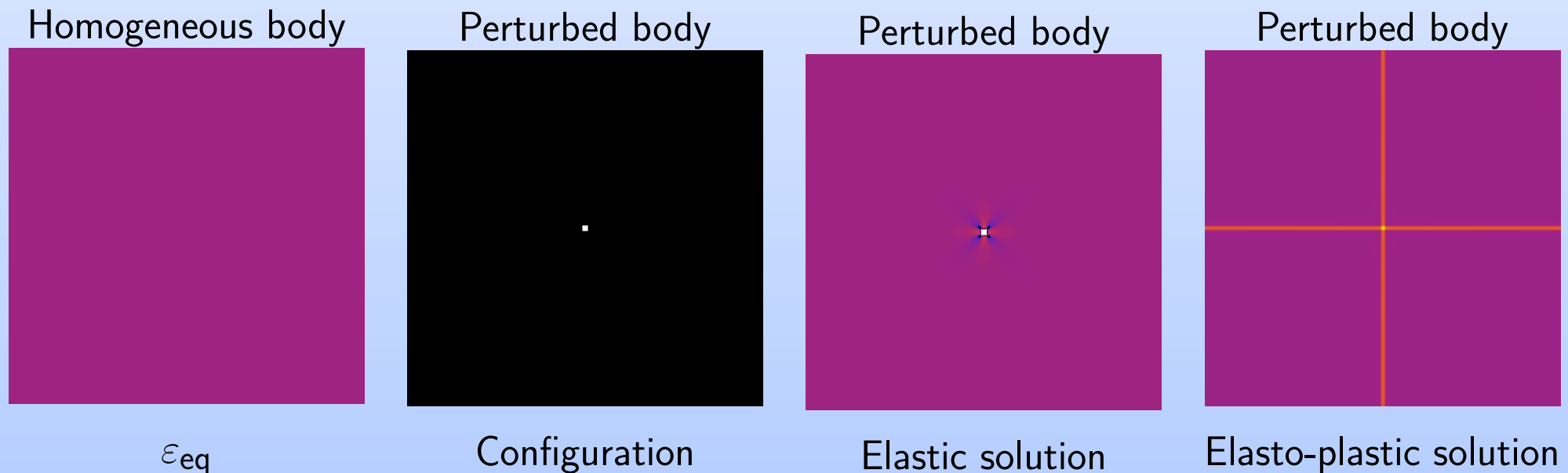
The Ugly (cont'd) : non-continuity with respect to data (Butterfly effect)

Simple shear on a block of elastic perfectly plastic material with periodic boundary conditions (simulations by H. Moulinec) :

Left, right side $u_2 = tx_1$, Top, bottom $u_1 = tx_2$.

Homogeneous body \Rightarrow homogeneous strain $\varepsilon_{12} = t$, other $\varepsilon_{ij} = 0$.

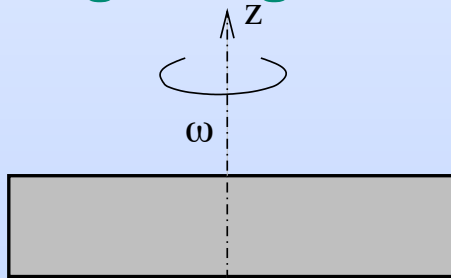
Perturbed body : On a tiny zone (volume fraction 0.027%) Young modulus = 0.95 initial modulus.
Same flow stress σ_0 everywhere.



Comments

- **Strictly positive hardening or viscosity** : unique and smooth solutions in the small strain setting. Only source of instability : large deformations resulting in **configuration changes**.
- **Inertia (dynamic problem instead of quasi-static)** restores uniqueness (but not smoothness). No safe-load condition necessary. **A plastic structure can be loaded beyond its (quasi-static limit load)** : the dynamic problem will continue to possess a solution !

Disk rotating at angular velocity ω



$$\operatorname{div}(\boldsymbol{\sigma}) + \rho\omega^2 r \mathbf{e}_r = 0, \quad \sigma_{\text{eq}} \leq \sigma_0 \Rightarrow \omega \leq \omega_{cr},$$

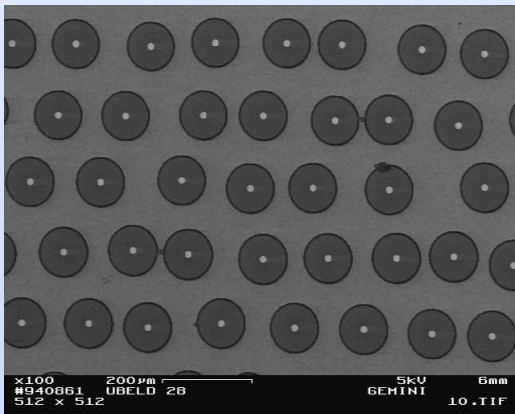
But solutions to the dynamic problem exist even when $\omega > \omega_{cr}$.

- Existence of a displacement field (re)-derived recently (2006) by Dal Maso *et al.* The proof is based on **Incremental Variational principles** (more about that later).

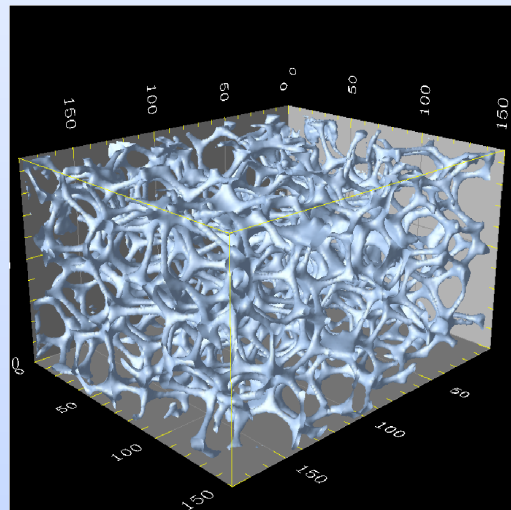
3. Upscaling. Homogenization

Question : Effective behaviour of heterogeneous material with elasto-plastic constituents at small scale ?

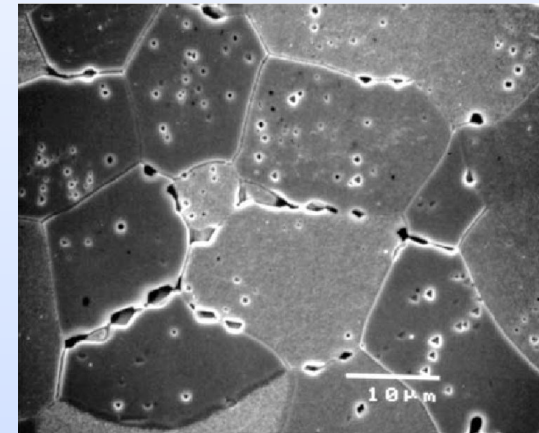
Virtually every material is heterogeneous at a sufficient small scale.



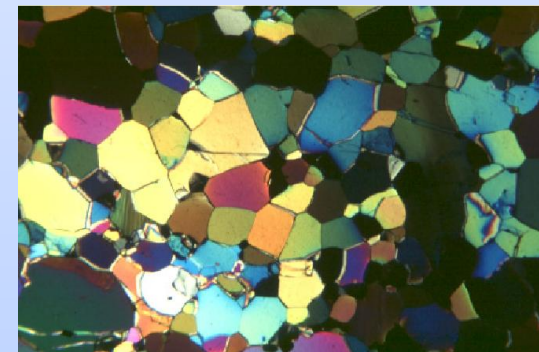
SiC/Ti



Metallic foam



UO₂

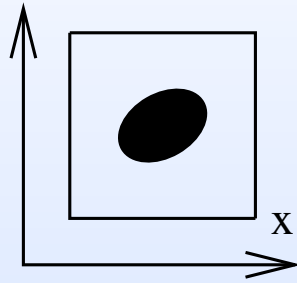


Ice

Composite materials : assemblage of different constituents (or phases) with different functions or properties. η **small parameter** related to the size of the heterogeneities.

Homogenization as an asymptotic procedure.

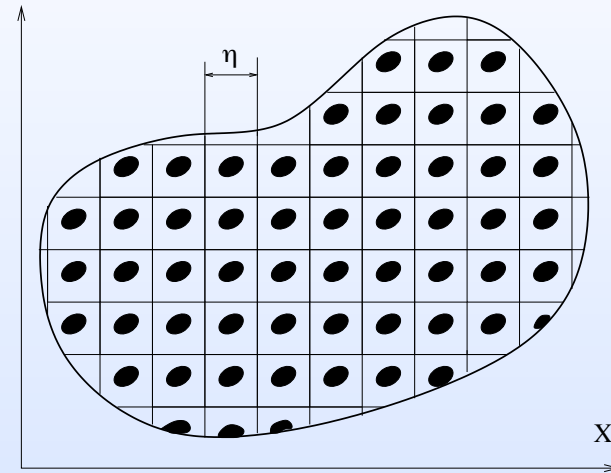
Periodic media



Unit-cell $V =]0, 1[{}^N$

$\chi_1(\mathbf{y})$ phase 1.

$$\mathbf{a}(\mathbf{y}) = \alpha \chi_1(\mathbf{y}) + \beta (1 - \chi_1(\mathbf{y})).$$



Domain Ω (cell size η)

$$\mathbf{a}^\eta(\mathbf{x}) = \mathbf{a}\left(\frac{\mathbf{x}}{\eta}\right) \text{ periodic with period } \eta.$$

Random media : χ_1 characteristic function of phase 1 = random variable.

Example of a linear homogenization problem :

$$\operatorname{div}(\boldsymbol{\sigma}^\eta)(\mathbf{x}) + f(\mathbf{x}) = \mathbf{0}, \quad \boldsymbol{\sigma}^\eta(\mathbf{x}) = \mathbf{a}^\eta(\mathbf{x}) \boldsymbol{\varepsilon}(\mathbf{u}^\eta(\mathbf{x})) \text{ in } \Omega + \text{B.C.}$$

$\mathbf{u}^0 = \lim_{\eta \rightarrow 0} \mathbf{u}^\eta$: homogenized field. BVP solved by \mathbf{u}^0 ?

Variety of convergence techniques

- **Multi-scale expansions for periodic media** (Sanchez-Palencia). Later rendered more rigorous by the two-scale convergence theory of Nguetseng and Allaire.
- **G -convergence** (De Giorgi -Spagnolo) : convergence of Green operators,
- **H -convergence** (Murat-Tartar), convergence of solutions,
- **Γ -convergence** (De Giorgi *et al*), convergence of energy,...

Typical Γ -convergence result :

Periodic media, p.d.e.'s derive from a (convex) energy w^η :

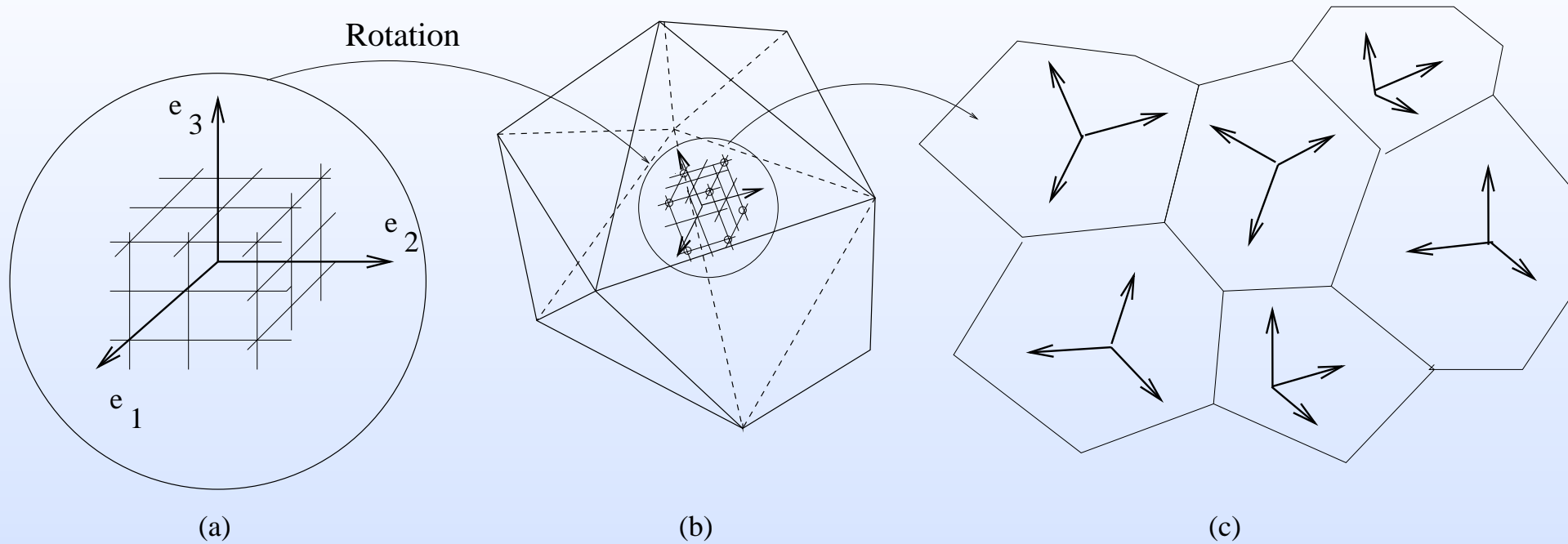
$$\boldsymbol{\sigma}^\eta = \frac{\partial w^\eta}{\partial \boldsymbol{\varepsilon}}(\mathbf{x}, \boldsymbol{\varepsilon}(\mathbf{u}^\eta)),$$

Then $\boldsymbol{\sigma}^\eta$ and \mathbf{u}^η converge (weakly in some functional space) to

$$\bar{\boldsymbol{\sigma}} = \frac{\partial \bar{w}}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}), \quad \bar{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon}(\bar{\mathbf{u}}).$$

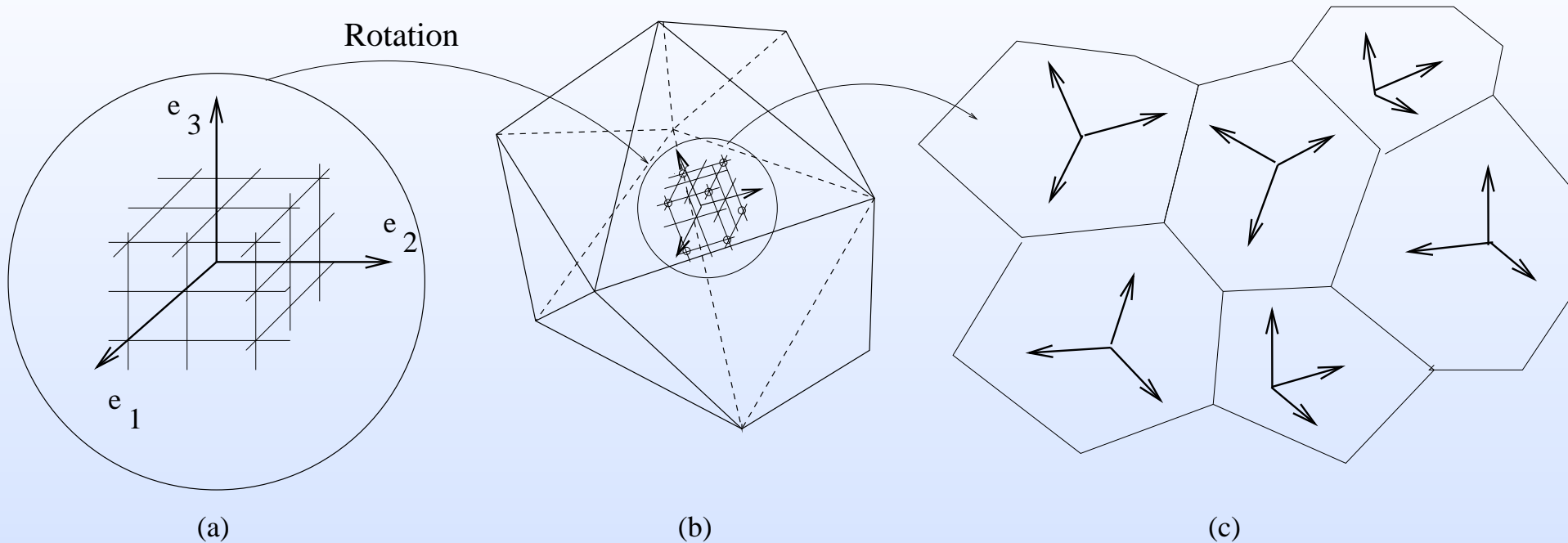
$$\bar{w}(\bar{\boldsymbol{\varepsilon}}) = \inf_{\mathbf{u} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \langle w(\mathbf{x}), \boldsymbol{\varepsilon}(\mathbf{u}) \rangle, \quad \langle \cdot \rangle = \frac{1}{|V|} \int_V \cdot \, d\mathbf{x}, \quad \mathcal{K}(\bar{\boldsymbol{\varepsilon}}) = \{\mathbf{u}, \mathbf{u} - \langle \boldsymbol{\varepsilon}(\mathbf{u}) \rangle \cdot \mathbf{x} \text{ periodic}\}$$

Polycrystal



Each grain is a copy of the same single crystal, with energy w^s except for its orientation θ which varies from grain to grain.

Polycrystal



Each grain is a copy of the same single crystal, with energy w^s except for its orientation θ which varies from grain to grain.

- Energy for the single crystal $w^s(\boldsymbol{\varepsilon})$.
- Energy for a rotated grain $w^s(\mathbf{R}, \boldsymbol{\varepsilon})$.
- **Effective energy for the polycrystal (aggregate of grains) :**

$$w^p(\bar{\boldsymbol{\varepsilon}}) = \inf_{\mathbf{u} \in \mathcal{K}(\bar{\boldsymbol{\varepsilon}})} \langle w^s(\mathbf{R}(\mathbf{x}), \boldsymbol{\varepsilon}(\mathbf{u})) \rangle .$$

Homogenization results for Rigid-plastic composites

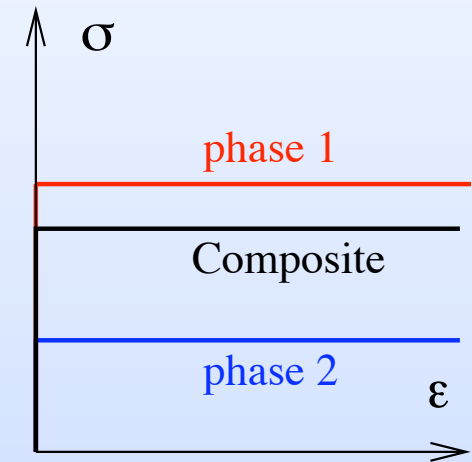
The Good

Rigid ideally plastic constituents, characterized by their flow surface :

$$\dot{\boldsymbol{\varepsilon}}^e = \mathbf{0}, \quad \boldsymbol{\sigma} = \frac{\partial d}{\partial \dot{\boldsymbol{\varepsilon}}}(\dot{\boldsymbol{\varepsilon}}).$$

Γ -convergence for convex functions which are positively homogeneous of degree 1 (Bouchitte-PS) : **there exists an effective flow surface :**

$$\tilde{d}(\dot{\boldsymbol{\varepsilon}}) = \inf_{\langle \dot{\boldsymbol{\varepsilon}} \rangle = \dot{\boldsymbol{\varepsilon}}} \langle d(\dot{\boldsymbol{\varepsilon}}) \rangle, \quad \tilde{d}(\lambda \dot{\boldsymbol{\varepsilon}}) = \lambda \tilde{d}(\dot{\boldsymbol{\varepsilon}}) \Rightarrow \tilde{d} = (I\tilde{P})^*$$



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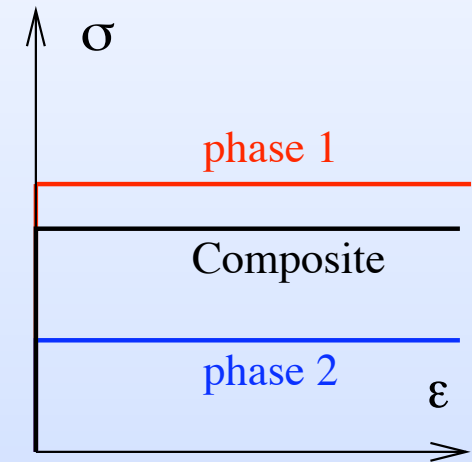
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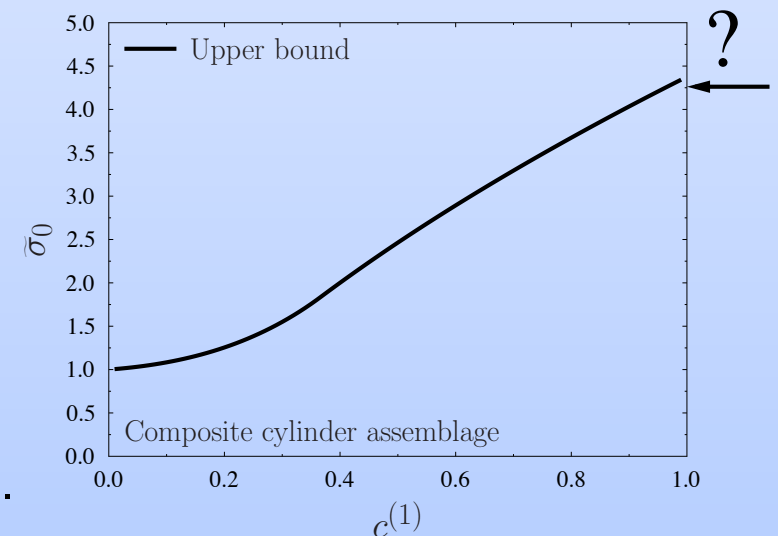
The Ugly

2-phase isotropic matrix-inclusion random composite,

$$\text{Inclusions : } \sigma_0^{(1)} = 5, \quad \text{Matrix : } \sigma_0^{(2)} = 1.$$

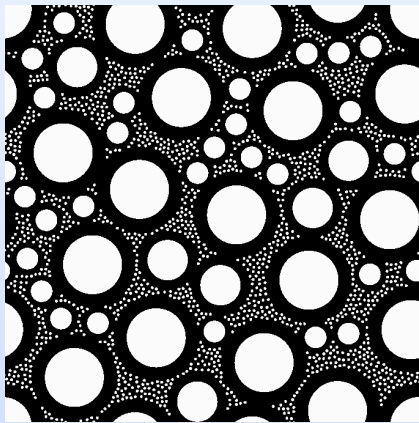
Effective properties are **usually continuous functions of the volume fraction :**

$$\sigma^{\text{hom}} = \sigma_0^{(2)} \text{ when } c^{(1)} = 0, \quad \text{OK,} \quad \sigma_0^{(1)} \text{ when } c^{(1)} = 1, \quad \text{NO.}$$

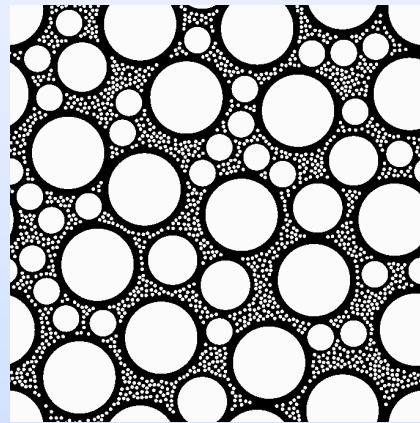


Plastic deformation under macroscopic shear (shear bands are at 0^0)

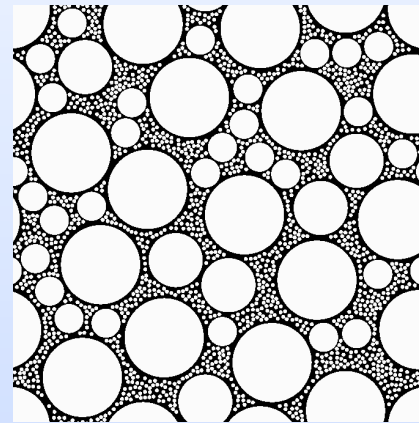
Simulations (H. Moulinec) at high volume fraction by filling up space with self-similar composite cylinders.



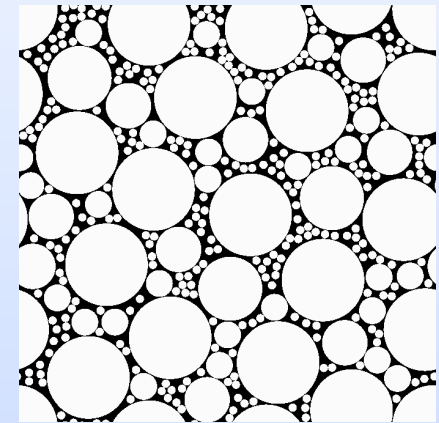
$$c^{(1)} = 0.43$$



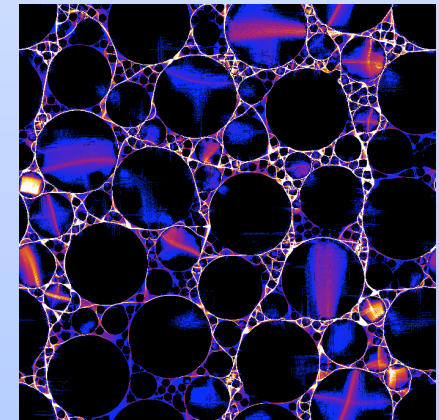
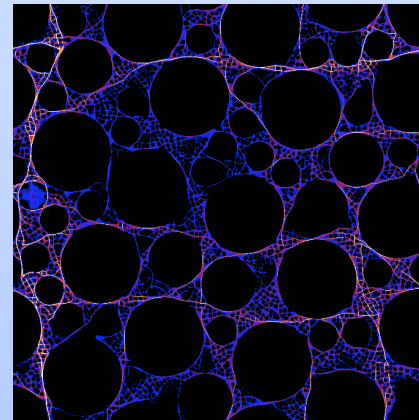
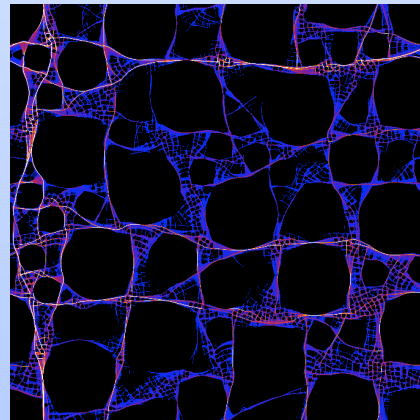
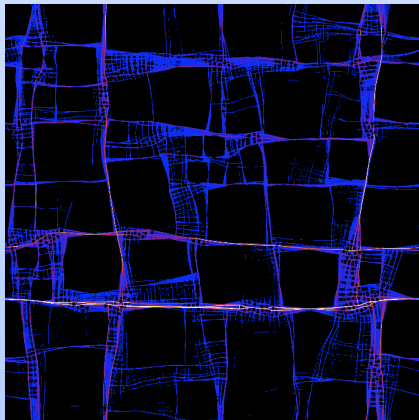
$$c^{(1)} = 0.65$$



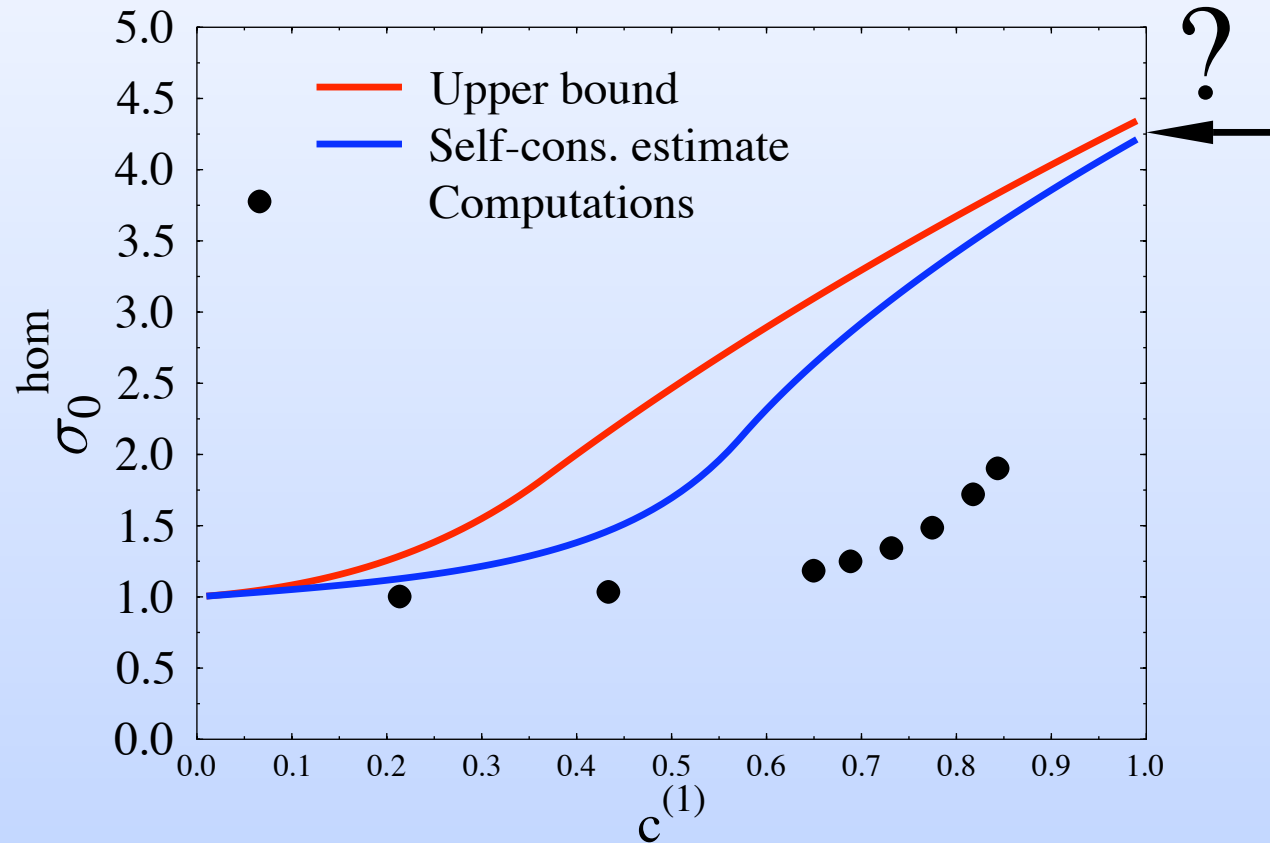
$$c^{(1)} = 0.775$$



$$c^{(1)} = 0.85$$



Effective properties

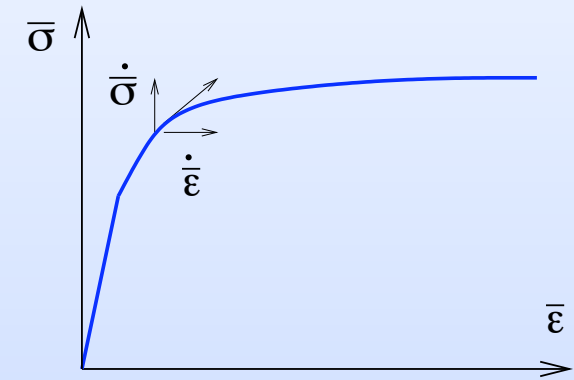
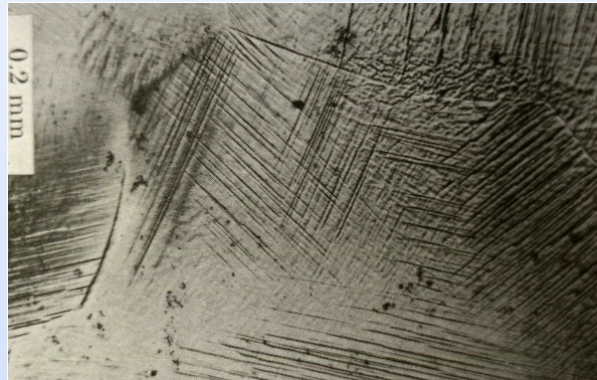
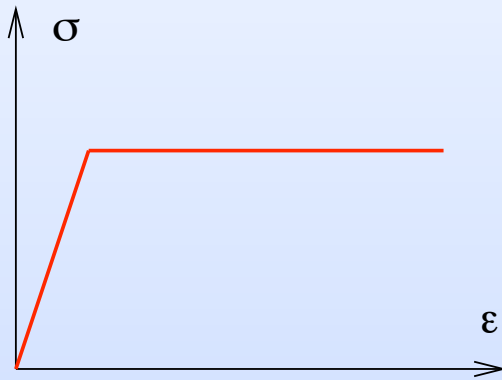


Plastic strain localizes in zones with zero volume fraction. A "memory" of the presence of the weakest phase persists in the limit $c^{(1)} \rightarrow 0$.

Homogenization results for **Elasto-plastic composites**

The Good

- **Elasto-plasticity can be homogenized.** Even though the local displacement field is not unique, the relation $(\bar{\sigma}, \bar{\epsilon})$ is uniquely defined.



- **Macroscopic hardening :**

$$\dot{\bar{\sigma}} : \dot{\bar{\epsilon}} = \langle \dot{\bar{\sigma}} : \dot{\bar{\epsilon}} \rangle = \langle \dot{\bar{\sigma}} : \mathbf{M} : \dot{\bar{\sigma}} \rangle + \langle \dot{\bar{\sigma}} : \dot{\bar{\epsilon}}^P \rangle, \quad \dot{\bar{\sigma}} : \mathbf{M} : \dot{\bar{\sigma}} \geq 0, \quad \dot{\bar{\sigma}} : \dot{\bar{\epsilon}}^P \geq 0.$$

- **Hardening of the individual constituents :** $\dot{\bar{\sigma}} : \dot{\bar{\epsilon}}^P \geq 0$ ($= 0$ in perfect plasticity).
- **Changes in stress :** $\dot{\bar{\sigma}} : \mathbf{S} : \dot{\bar{\sigma}} \geq 0$. Remains > 0 as long as there is a change in the stress field (expansion of the plastic zone, rotation of the stress).

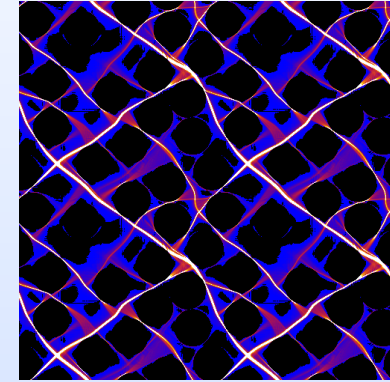
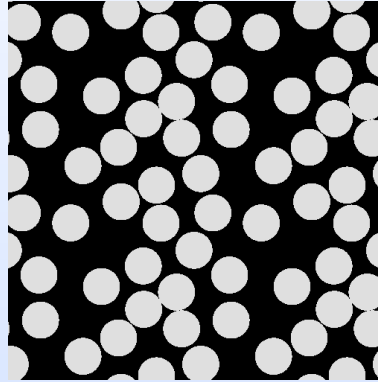
Localization and intermittency are more likely to be observed at small scale and not necessarily at the largest scale. They are (partially) smeared out by upscaling.

The Bad

- The statistics of the local strain field is NOT unique. Local details matter. Long range effects.
Tension at 0^0

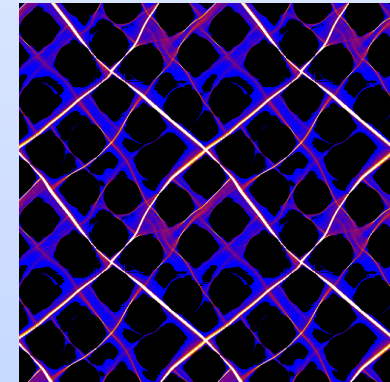
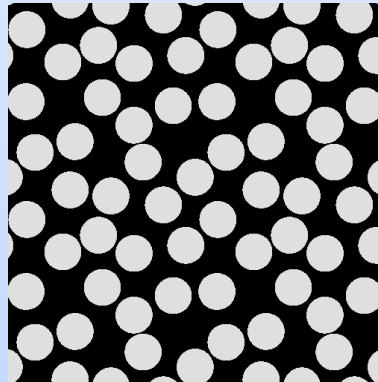
“Hard” configuration.

Locking of shear bands by clusters of fibers.
Clusters play a favourable role to prevent strain localization.



“High” flow stress.

“Weak” configuration. More regular spatial arrangement. Shear bands running at $\pm 45^0$ with respect to the tensile direction.



“Low” flow stress.

Percolation of shear bands.

The composite effective properties are not governed by the volume fraction of the fibers but by the tortuosity of the matrix domain.

- The size of the representative volume element is an open question (how many grains, inclusions?).

The Ugly : description of the macroscopic hardening through effective constitutive relations

Homogenization of highly heterogeneous materials with nonlinear dissipative constituents entering the class of *Generalized Standard Materials (GSM)* (Halphen & Nguyen, 1975) governed by two convex potentials w free-energy, φ dissipation potential :

At each point x of the (micro)structure :

State of the system (state variables) : $\boldsymbol{\varepsilon}, \boldsymbol{\alpha} = \boldsymbol{\varepsilon}^p,$

Energy available in the system : $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}),$

\Rightarrow **Driving forces** : $\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}), \quad \mathcal{A} = -\frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}),$

Evolution of the internal variables : $\mathcal{A} = \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) \Leftrightarrow \dot{\boldsymbol{\alpha}} = \frac{\partial \varphi^*}{\partial \mathcal{A}}(\mathcal{A}).$

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}), \quad \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) + \frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = 0.$$

Example 1 : von Mises Plasticity

State variables : $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}^p,$

Free energy : $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) : \mathbf{M} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p)$

Dissipation potential : $\varphi(\dot{\boldsymbol{\alpha}}) = \sigma_0 \dot{\varepsilon}_{eq}^p.$

Example 2 : Crystalline Plasticity

State variables : $\boldsymbol{\alpha} = \{ \gamma^{(k)}, k = 1, \dots, N \},$

Free energy : $w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) = \frac{1}{2} \left(\boldsymbol{\varepsilon} - \sum_{k=1}^N \gamma^{(k)} \boldsymbol{\mu}^{(k)} \right) : \mathbf{M}^e : \left(\boldsymbol{\varepsilon} - \sum_{k=1}^N \gamma^{(k)} \boldsymbol{\mu}^{(k)} \right),$

Dissipation potential : $\varphi(\dot{\boldsymbol{\alpha}}) = \sum_{k=1}^N \tau_0^{(k)} |\dot{\gamma}^{(k)}|.$

EXACT separation of scales in nonlinear problems is NOT met : an infinite number of internal variables is required (Mandel 68, Rice 71, PS 82, justified recently for elasto-viscoplasticity by two-scale convergence, Visintin 2006).

State variables	:	$\bar{\boldsymbol{\varepsilon}}, \quad \bar{\boldsymbol{\alpha}} = \{\boldsymbol{\varepsilon}^P(\boldsymbol{x})\}_{\boldsymbol{x} \in V},$
Potentials	:	$\bar{w}(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\alpha}}) = \langle w(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^P) \rangle, \quad \bar{\varphi}(\dot{\bar{\boldsymbol{\alpha}}}) = \langle \varphi(\dot{\boldsymbol{\varepsilon}}^P) \rangle,$
Driving forces	:	$\bar{\boldsymbol{\sigma}} = \frac{\partial \bar{w}}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\alpha}}), \quad \bar{\boldsymbol{\mathcal{A}}} = -\frac{\partial \bar{w}}{\partial \bar{\boldsymbol{\alpha}}}(\bar{\boldsymbol{\varepsilon}}, \bar{\boldsymbol{\alpha}}),$
Evolution of internal variables	:	$\bar{\boldsymbol{\mathcal{A}}} = \frac{\partial \bar{\varphi}}{\partial \dot{\bar{\boldsymbol{\alpha}}}}(\dot{\bar{\boldsymbol{\alpha}}}).$

⇒ **At each macroscopic point X , the entire field of the microscopic internal variables $\{\boldsymbol{\varepsilon}^P(\boldsymbol{x})\}_{\boldsymbol{x} \in V}$ in the volume V has to be determined.** No scale decoupling.

Results from the interplay between elasticity and dissipation (the same result holds for linearly viscous, or nonlinearly viscous materials).

Approximate models

- Model reduction (P.O.D. with JC Michel) : **Non Uniform Transformation Field Analysis.**
- **Variational approximations** (with N. Lahellec).

Variational approximation

Reduction from two potentials to a one potential for a single phase

$$\sigma = \frac{\partial w}{\partial \varepsilon}(\varepsilon, \alpha), \quad \frac{\partial \varphi}{\partial \dot{\alpha}}(\dot{\alpha}) + \frac{\partial w}{\partial \alpha}(\varepsilon, \alpha) = 0.$$

Incremental variational principles (Mialon, 1986, Ortiz & Stainier, 1999, Miehe, 2002...)

- Upon time discretization $[0, T] : t_0 = 0, t_1, \dots, t_N = T$.

$$\sigma_n = \sigma(t_n), \dots$$

- Euler backward time-integration :

$$\sigma_{n+1} = \frac{\partial w}{\partial \varepsilon}(\varepsilon_{n+1}, \alpha_{n+1}), \quad \frac{\partial \varphi}{\partial \dot{\alpha}}\left(\frac{\alpha_{n+1} - \alpha_n}{\Delta t}\right) + \frac{\partial w}{\partial \alpha}(\varepsilon_{n+1}, \alpha_{n+1}) = 0.$$

Condensed potential : $\sigma, \varepsilon \dots$ stand for $\sigma_{n+1}, \varepsilon_{n+1}, \dots$:

$$\sigma = \frac{\partial w_{\Delta}}{\partial \varepsilon}(\varepsilon),$$

$$w_{\Delta}(\varepsilon) = \inf_{\alpha} J(\varepsilon, \alpha), \quad \text{with} \quad J(\varepsilon, \alpha) = w(\varepsilon, \alpha) + \Delta t \varphi\left(\frac{\alpha - \alpha_n}{\Delta t}\right).$$

Incremental Variational Principle

N -phase heterogeneous material : phase r with potentials $w^{(r)}, \varphi^{(r)}$

$$\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle = \frac{\partial \tilde{w}_\Delta}{\partial \bar{\boldsymbol{\varepsilon}}}(\bar{\boldsymbol{\varepsilon}}), \quad \tilde{w}_\Delta(\bar{\boldsymbol{\varepsilon}}) = \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}} \langle w_\Delta(\boldsymbol{\varepsilon}) \rangle = \inf_{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}} \left\langle \inf_{\boldsymbol{\alpha}} J(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) \right\rangle,$$

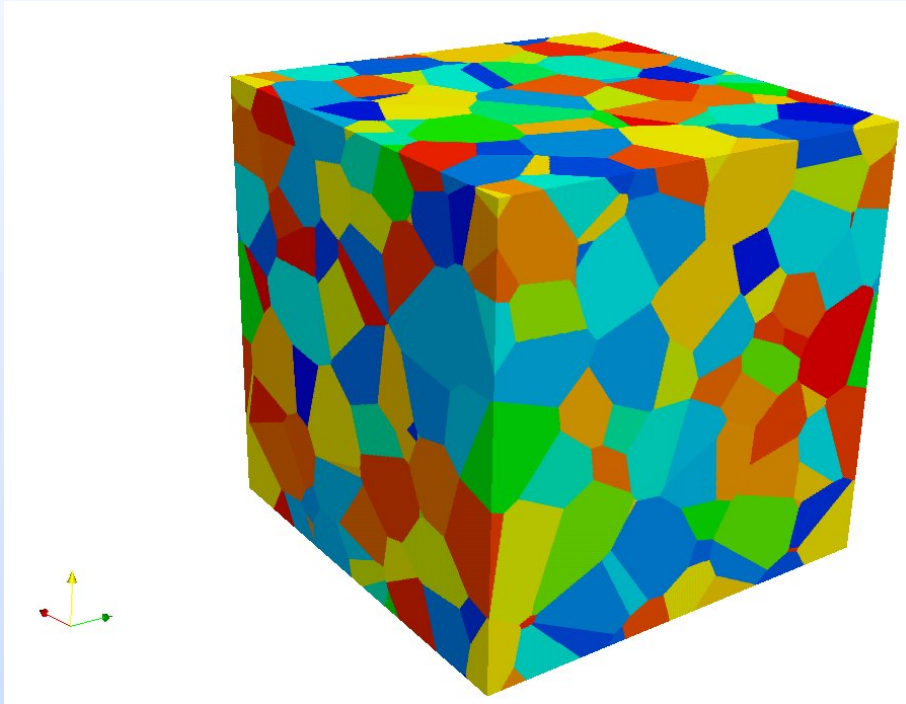
$$J(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}, \boldsymbol{x}) = w^{(r)}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \Delta t \varphi^{(r)} \left(\frac{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n(\boldsymbol{x})}{\Delta t} \right) \text{ in phase } r.$$

Two major obstacles :

- **φ is nonquadratic** : **Must be LINEARIZED** (as in nonlinear homogenization) : approximate (optimally in a variational sense) a nonlinear composite, by a linear (thermoelastic) comparison composite (J. Willis, P. Ponte Castañeda, PS). Analytical results available for the effective properties of the LCC (Hashin-Shtrikman, self-consistent...).
- **$\boldsymbol{\alpha}_n(\boldsymbol{x})$ is a FIELD. Must be replaced by an EFFECTIVE INTERNAL VARIABLE $\boldsymbol{\alpha}_n^{(r)}$.** $\boldsymbol{\alpha}_n^{(r)}$ should capture the statistics of the field $\boldsymbol{\alpha}_n(\boldsymbol{x})$ (even when both w and φ are quadratic, linear viscoelasticity).

NB : Lahellec & PS (2007) have proposed a "variational" approximation of J by a quadratic potential J_0 (again a linear thermoelastic comparison composite). $\boldsymbol{\alpha}_n^{(r)}$ depends on the first and second moment of $\boldsymbol{\alpha}_n(\boldsymbol{x})$ in phase r (UGLY in P.P.).

Polycrystals



300 grains with random orientation.

Self-consistent : accurate prediction for the effective properties of polycrystals with random orientation (and shape) of the grains.

Elastic properties.

Single crystal elastic properties (GPa)

	C_{11}	C_{12}	C_{33}	C_{13}	C_{44}
Copper (cubic)	171	122	$= C_{11}$	$= C_{12}$	69.1
Zinc (hexagonal)	163.4	36.4	53.	63.5	38.8

Polycrystal effective properties

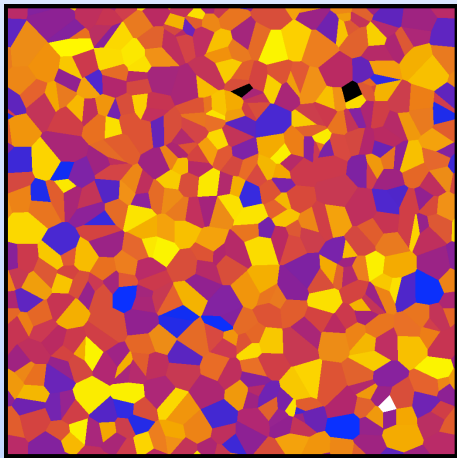
	k FFT	k SC	k meas.	μ FFT	μ SC	μ meas.
Cu	138.3	138.3	138	46.4	46.3	45.5
Zn	70.54	70.9	68.5	40.7	40.6	41.2

Elasto-Viscoplastic polycrystals

N -phase composite material with $N =$ number of family of orientations.

Model problem : Anti-plane

$$\mathbf{u} = u_3(x_1, x_2)\mathbf{e}_3, \quad \varepsilon_{13}, \quad \varepsilon_{23}, \quad \sigma_{13}, \quad \sigma_{23} \neq 0, \quad \text{other } \varepsilon_{ij}, \sigma_{ij} = 0.$$



10 configurations with
500 grains

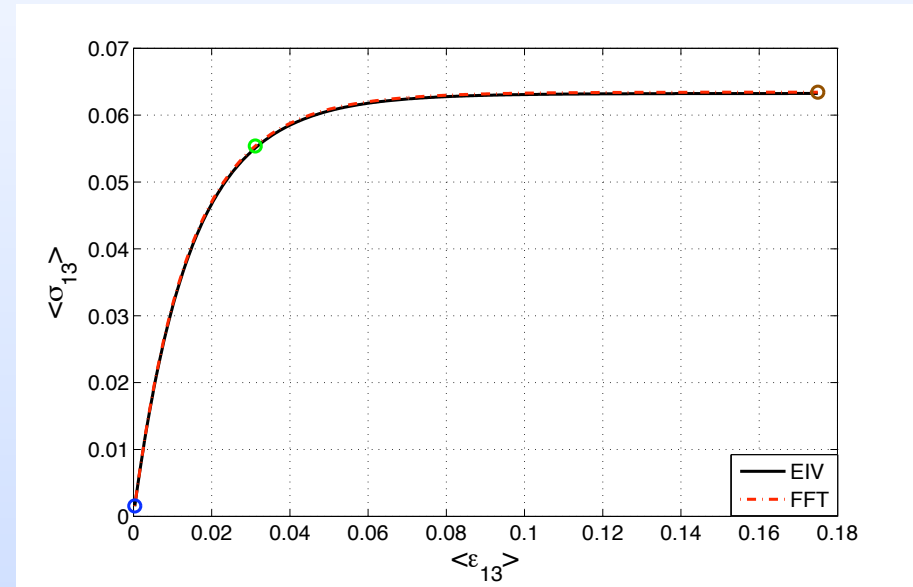
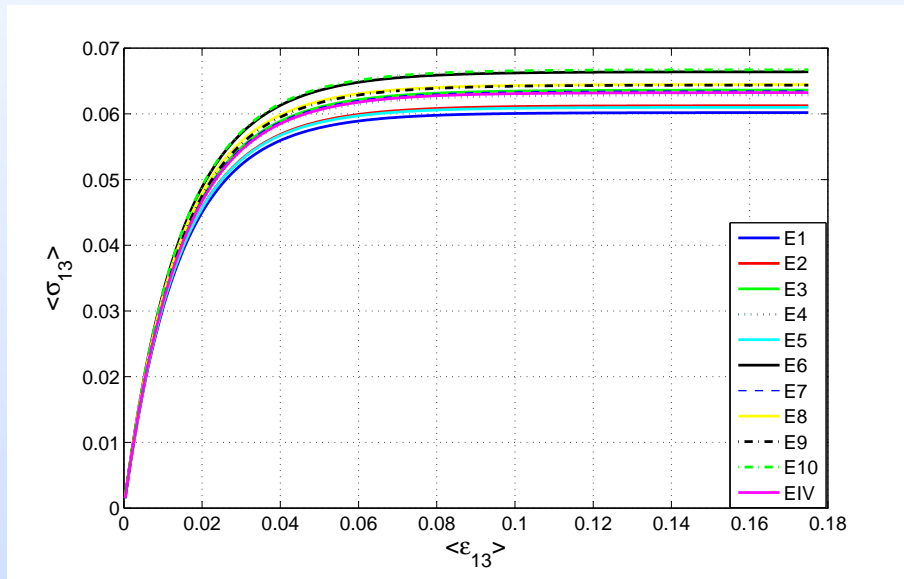
- Each grain has a different orientation $\theta^{(r)}$:
 $(\mathbf{e}_1^{(r)}, \mathbf{e}_2^{(r)})$ rotated from $(\mathbf{e}_1, \mathbf{e}_2)$ by $\theta^{(r)}$.
- 2 orthogonal slip systems

$$\boldsymbol{\mu}^{(1,r)} = \frac{1}{2}(\mathbf{e}_1^{(r)} \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1^{(r)}), \quad \boldsymbol{\mu}^{(2,r)} = \frac{1}{2}(\mathbf{e}_2^{(r)} \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2^{(r)}).$$

- Loading : monotone loading at constant strain-rate :

$$\bar{\varepsilon}_{13}(t) = \dot{\varepsilon}_0 t, \quad \bar{\varepsilon}_{23}(t) = 0.$$

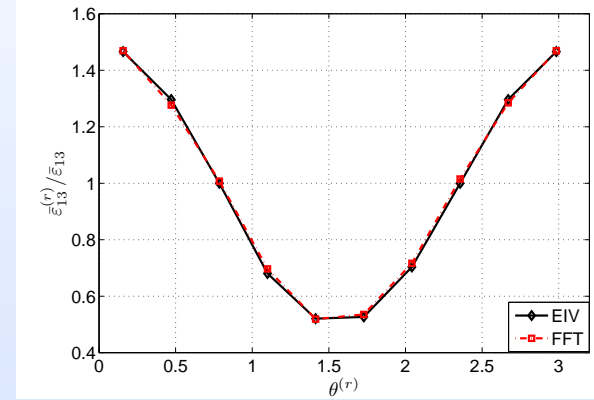
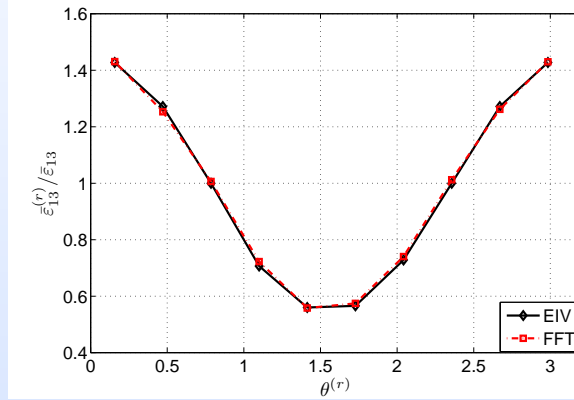
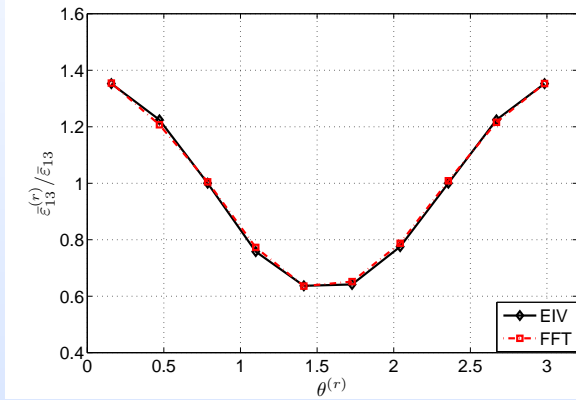
Linear Viscoelasticity : $n^{(k)} = 1$



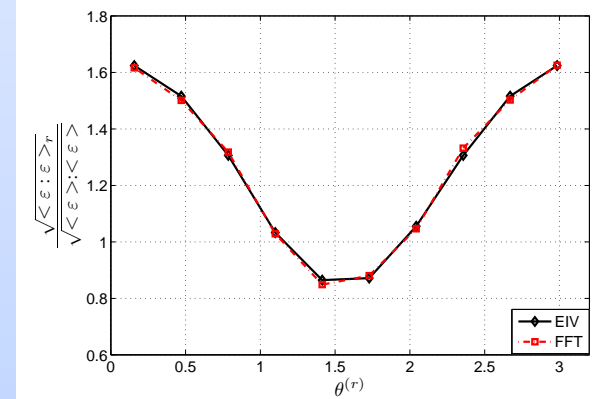
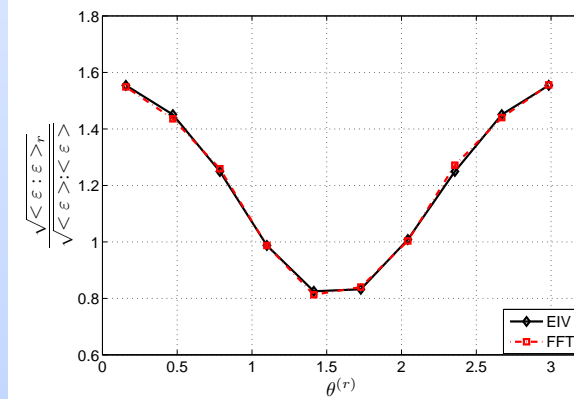
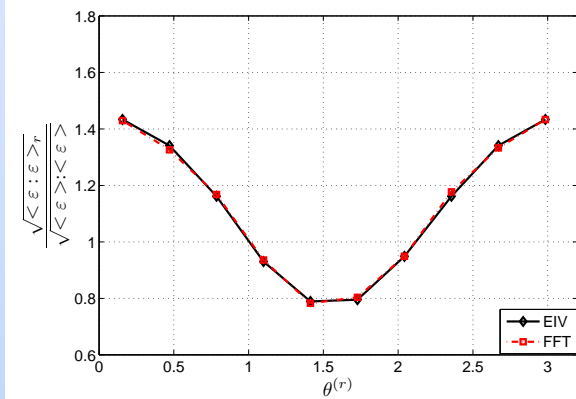
- Taking the ensemble average over 10 configurations of 500 grains seems to be enough to achieve representativity (in this particular example) .
- Excellent agreement between the full-field simulations and the EIV (effective internal variable) model.
- **Statistics of the local fields?** At different times of the loading history : initial (elastic), transient, asymptotic (purely viscous) ?

First and second moments of the strain field.

1st



2nd

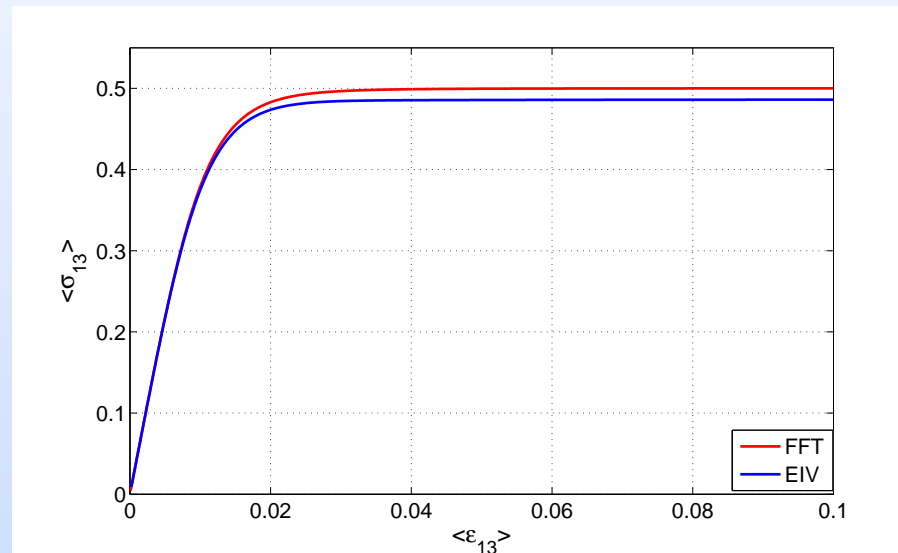


**Initial response
(elastic)**

**Transient response
(viscoelastic)**

**Asymptotic response
(purely viscous)**

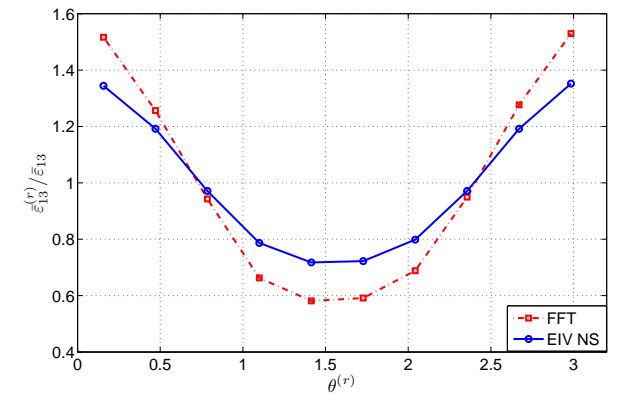
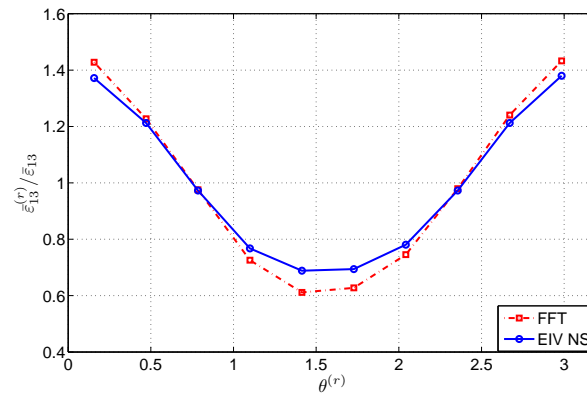
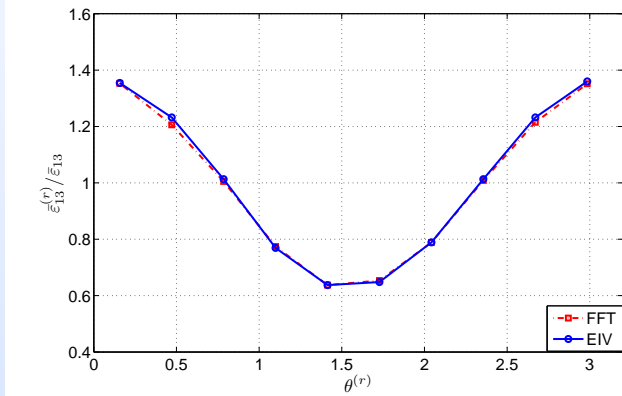
Nonlinear Elasto-Viscoplasticity : $n = 3$



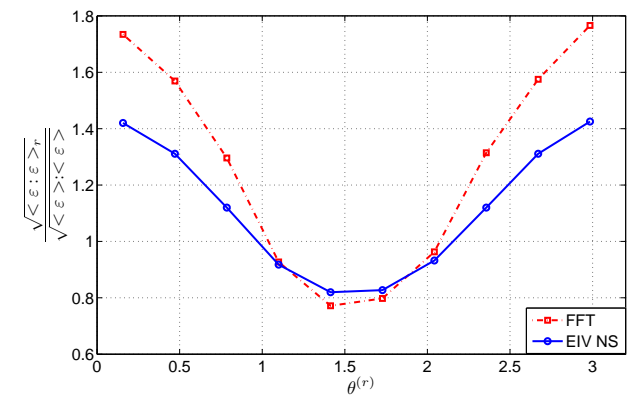
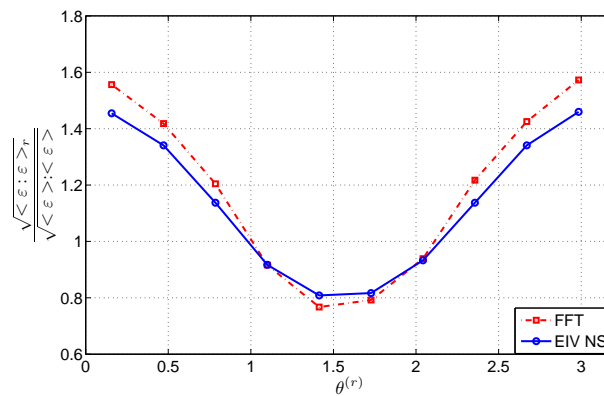
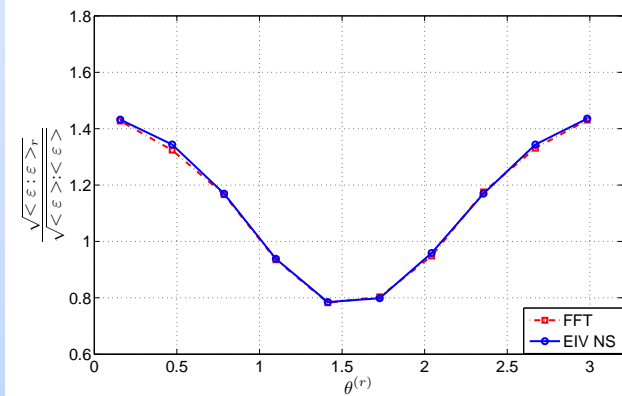
- **Linearization technique : variational (also called "modified secant").** Known to be too stiff (rigorous upper bound).
- The error in the transient regime is comparable to that in the asymptotic regime.

First and second moments of the strain field.

1st



2nd



Initial response
(elastic)

Transient response
(elasto-viscoplastic)

Asymptotic response
(purely viscous)

Conclusions

- The main features of plastic deformation at small scale, **intermitency and localization**, are well captured by elastic perfectly plastic crystalline models.
- Provided that there is no change in configuration, **upscaling stabilizes the material**. The overall stress-strain response is less jerky and exhibits (partial) positive hardening.
- The exact description of this hardening is a complicated task.
- Approximate models are under development. **Incremental Variational Principles**, coupled with nonlinear homogenization techniques are promising to make rational approximations.