Numerical simulations for nonlinear composites

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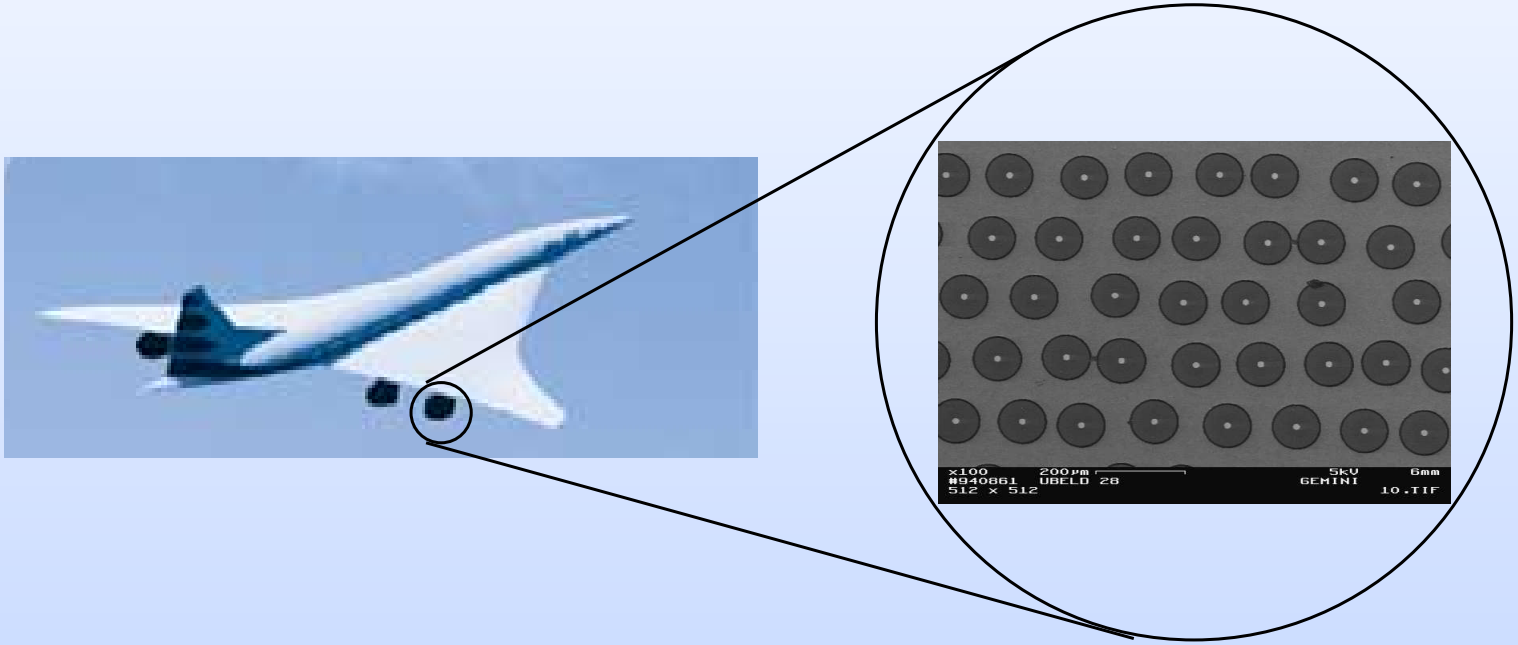
Draws from joint work with :
K. Bhattacharya (Caltech), J.C. Michel (Marseille),
P. Ponte Castañeda (Philadelphia, Paris) .

1. Outline



Several scales are present in the problem.

Should it be treated as “multiscale” problem ?

Terminology used in this talk

- **Multiscale problem :** a problem in which several length-scales are coupled and must be resolved simultaneously.
- **"Homogenization" or upscaling problem :** a problem in which the scales are well separated and do not need to be resolved at the same time (change of scales).
- **Homogenization for linear problems : OK : The problem at the macroscopic scale and at the microscopic scales are uncoupled**

$$\boldsymbol{\sigma} = \boldsymbol{L}(x) : \varepsilon, \quad \overline{\boldsymbol{\sigma}} = \widetilde{\boldsymbol{L}} : \overline{\varepsilon},$$

  where $\widetilde{\boldsymbol{L}}$ is known by solving, once for all, 6 elasticity problems.
- **Homogenization for nonlinear problems : theoretically feasible but remains a multiscale problem !** Even when the scales are well separated, the macroscopic problem and the microscopic problem are coupled.

Ultimate goal : Avoid Multiscale problems ! Introduce approximations to decouple the scales or reduce the coupling to only a few "microstructural variables".

Composite materials are ubiquitous in nature and in man-made structures.

Aim of this talk : discuss the local and global response of nonlinear composites

1. Computationally : address composites with complex microstructure.

$\Rightarrow$ **Fast numerical method for elliptic p.d.e.'s with periodicity conditions.**

2. Theoretically : assess the accuracy of theoretical bounds or estimates for (nonlinear) composites.

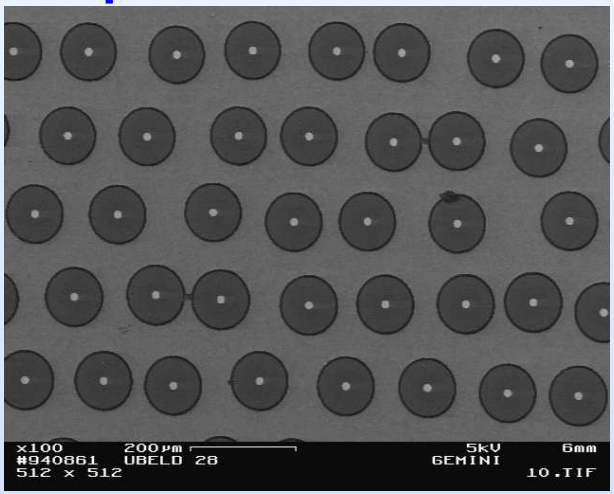
$\Rightarrow$ **Importance of intraphase field heterogeneity**.

3. Approximate models : make approximations under which the multiscale problem for nonlinear composites can decoupled.

$\Rightarrow$ **Nonuniform transformation field analysis**.

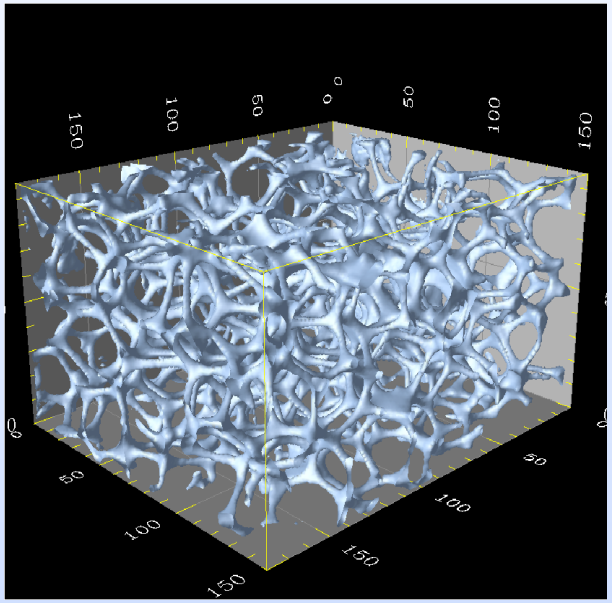
Composites with complex microstructure

Simple microstructure

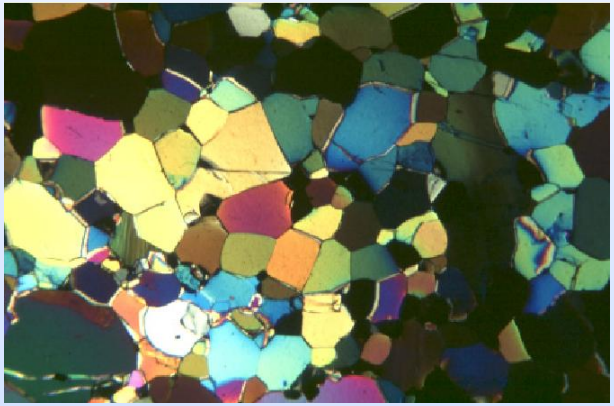


SiC-Ti (ONERA)

Complex microstructures



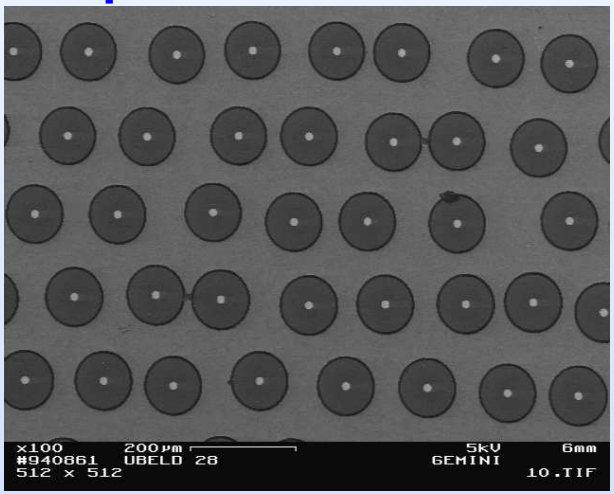
Metallic foam (GEMPPM)



Polycrystal

Composites with complex microstructure

Simple microstructure



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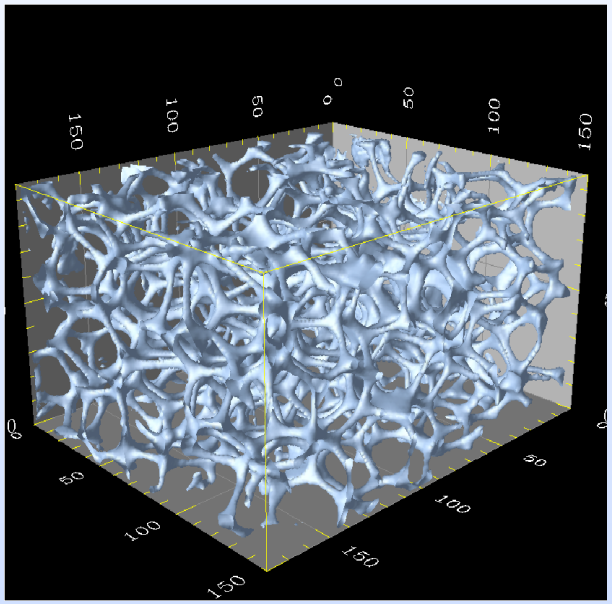

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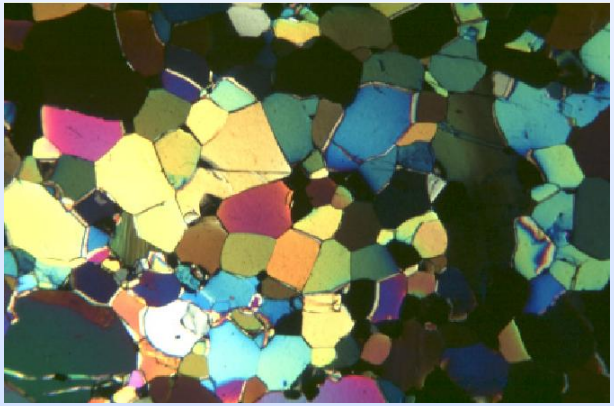


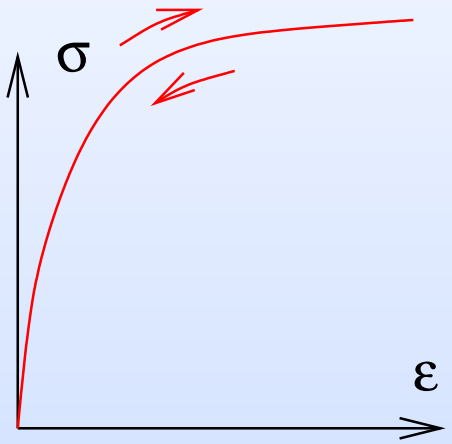
Polycrystal

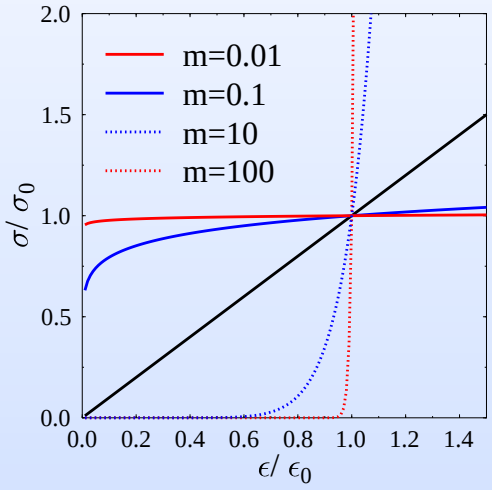
Compute the effective properties and the local response of composites with complex microstructures. Make use of *images of their real microstructure.*

Local fields : High spatial resolution required : large number of dof's. Large systems.

Nonlinear phases

Nonlinear elasticity : $\boldsymbol{\sigma = f(\varepsilon)}$





Power-law materials :

$$\mathrm{tr}\varepsilon = 0, \quad \frac{\sigma}{\sigma_0} = \left(\frac{\varepsilon}{\varepsilon_0}\right)^m .$$

$m = 1$: Linear elastic materials,

$m = 0$: rigid-plastic materials,

$m = +\infty$: adaptative materials.

Nonlinear phases

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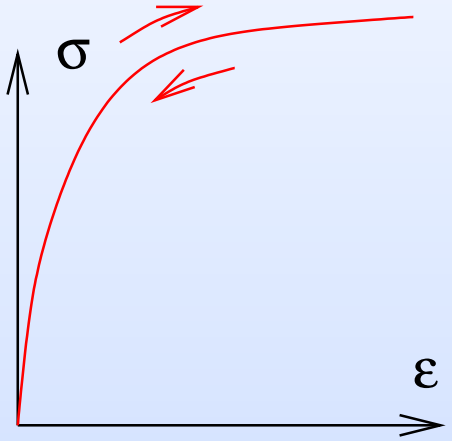

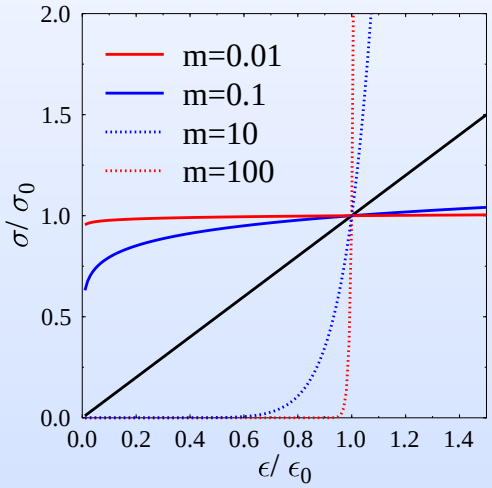

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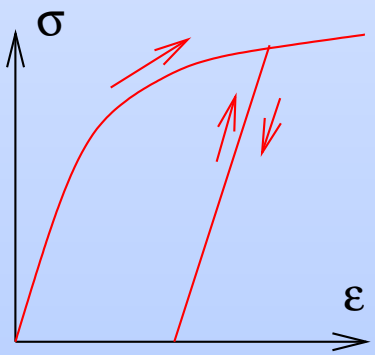
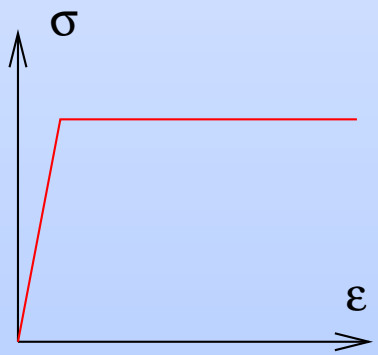
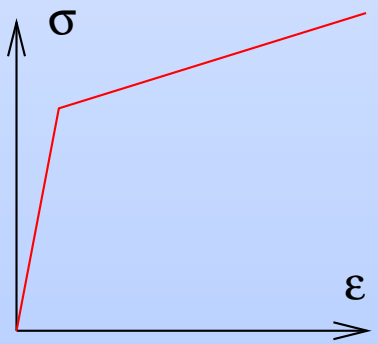
Incremental plasticity : $\boldsymbol{\varepsilon} = \boldsymbol{M} : \boldsymbol{\sigma} + \boldsymbol{\varepsilon}^{\mathrm{p}}, \quad \dot{\boldsymbol{\varepsilon}}^{\mathrm{p}} = \partial\psi/\partial\boldsymbol{\sigma}(\boldsymbol{\sigma}).$:





Perfect plasticity

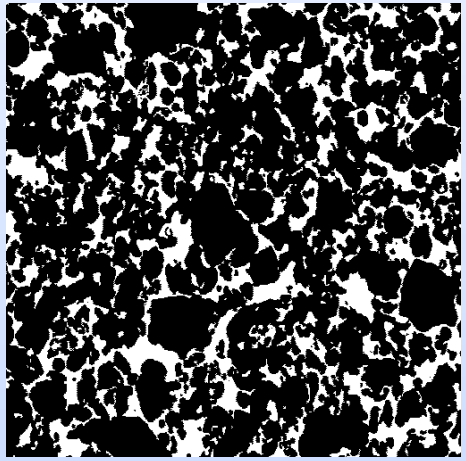


Plasticity with linear hardening

2. A computational method for composites

based on Fast Fourier Transforms... Moulinec and Suquet (1994), W. Muller (1996), Eyre and Milton (1999), Lebensohn (2000)...

Required input :



- **Constitutive relations** for the phases (including interfaces). $\boldsymbol{\sigma}$, ε stress and infinitesimal tensors :

$$\boldsymbol{\sigma}(x) = \mathcal{F}(x, \varepsilon(x), \dot{\varepsilon}(x)....).$$

- **Microstructure.** Only partial statistical information available. Ensembble averaging over several realizations.
- **Boundary conditions** representing the *in situ* state of the rve.

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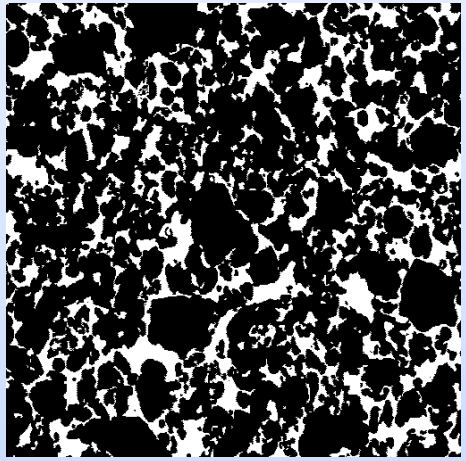

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Expected output :

- **Homogenized constitutive relations :**

$$\overline{\boldsymbol{\sigma}} = \widetilde{\mathcal{F}}(\overline{\varepsilon}, \dot{\overline{\varepsilon}}, ...) \quad ?$$

  where overall (macroscopic) strain, stress $\overline{\varepsilon} = \langle \varepsilon \rangle, \overline{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle$, $\langle . \rangle$ spatial averaging
- **Local fields** : $\boldsymbol{\sigma}$, ε. How heterogeneous are they ?

Local problem

$\boldsymbol{\sigma}(\boldsymbol{x}) = \mathcal{F}(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{x}), \dot{\boldsymbol{\varepsilon}}(\boldsymbol{x}) \ldots)$	**Constitutive relations**
$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\boldsymbol{\nabla u} + {}^{\mathsf{T}}\boldsymbol{\nabla u}\right)$	**Compatibility**
$\operatorname{div}(\boldsymbol{\sigma}) = 0$	**Equilibrium**
$\langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}$	**Loading**
$\boldsymbol{u}^* = \boldsymbol{u} - \overline{\boldsymbol{\varepsilon}}.\boldsymbol{x}$ periodic, $\boldsymbol{\sigma}.\boldsymbol{n}$ anti-periodic	**Boundary conditions**

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Constitutive relations : **ordinary differential equations** (NO coupling between material points).

Equilibrium + compatibility : **partial differential equations** (coupling between material points).

Eshelby's auxiliary problem

V representative volume element, **homogeneous reference medium** with elastic stiffness $\boldsymbol{L}^0$ subject to a nonhomogeneous eigenstress $\boldsymbol{\tau}$ (transformation stress)

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}^0 : \boldsymbol{\varepsilon}(\boldsymbol{u}^*(\boldsymbol{x})) + \boldsymbol{\tau}(\boldsymbol{x}), \quad \operatorname{div}(\boldsymbol{\sigma}) = 0, \quad \langle \boldsymbol{\varepsilon}(\boldsymbol{u}^*) \rangle = 0, \quad \textbf{Periodicity conditions}.$$

$$\Rightarrow \quad \boxed{\boldsymbol{\varepsilon}(\boldsymbol{u}^*(\boldsymbol{x})) = -\boldsymbol{\Gamma}^0 * \boldsymbol{\tau}(\boldsymbol{x}), \quad \widehat{\boldsymbol{\varepsilon}}^*(\boldsymbol{\xi}) = -\widehat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \widehat{\boldsymbol{\tau}}(\boldsymbol{\xi}) \ \ \forall \boldsymbol{\xi} \neq \boldsymbol{0}, \quad \widehat{\boldsymbol{\varepsilon}}^*(\boldsymbol{0}) = \boldsymbol{0}.}$$

$\boldsymbol{\Gamma}^0$: Green's operator for the reference medium.

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$\boldsymbol{\Gamma}^0$: Green's operator for the reference medium.

Properties of $\boldsymbol{\Gamma}^0$:

- $\boxed{\boldsymbol{\Gamma}^0 * \boldsymbol{\tau} = \boldsymbol{0} \ \Leftrightarrow \ \operatorname{div}(\boldsymbol{\tau}) = 0.}$ $\boldsymbol{\Gamma}^0 * \boldsymbol{\tau}$ measures the "distance" to equilibrium.
- $\boldsymbol{\Gamma}^0 * \boldsymbol{\tau}$ is a **compatible fluctuation field** $\forall \boldsymbol{\tau}$.
- $\boxed{\boldsymbol{\Gamma}^0 * \left(\boldsymbol{L}^0 : \boldsymbol{\varepsilon}(\boldsymbol{u})\right) = \boldsymbol{\varepsilon}(\boldsymbol{u}^*).}$

$\boldsymbol{\Gamma}^0$ is a (nonorthogonal) projector on compatible fluctuation fields.

Green's operator

Standard Fourier analysis : Willis, 64, Khatchaturyan, 73, Mura, 82.

$$\frac{\partial f}{\partial x_j} \overset{\text{Fourier}}{\rightarrow} \mathrm{i}\xi_j \widehat{f}(\boldsymbol{\xi}) \quad \mathrm{i} = \sqrt{-1}, \quad \mathrm{div}(\boldsymbol{\sigma}) = 0 \rightarrow \mathrm{i}\,\boldsymbol{\xi}.\widehat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) = 0, \quad \nabla \boldsymbol{u} \rightarrow \mathrm{i}\boldsymbol{\xi} \otimes \widehat{\boldsymbol{u}}(\boldsymbol{\xi}) \ldots.$$

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Isotropic reference medium :

$$\hat{\Gamma}^0_{ijkh}(\boldsymbol{\xi}) = \frac{1}{4\mu^0|\boldsymbol{\xi}|^2}(\delta_{ki}\xi_h\xi_j + \delta_{hi}\xi_k\xi_j + \delta_{kj}\xi_h\xi_i + \delta_{hj}\xi_k\xi_i) - \frac{\lambda^0 + \mu^0}{\mu^0(\lambda^0 + 2\mu^0)} \frac{\xi_i\xi_j\xi_k\xi_h}{|\boldsymbol{\xi}|^4}.$$

Back to initial problem

Linear elasticity :

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : \varepsilon(\boldsymbol{x}), \quad < \varepsilon >= \overline{\varepsilon}, \quad \varepsilon = \varepsilon(\boldsymbol{u}^*) + \overline{\varepsilon},$$

re-written as : $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}^0 : \varepsilon(\boldsymbol{u}^*(\boldsymbol{x})) \; + \; \boldsymbol{\tau}(\boldsymbol{x})$, with

$$\boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{\delta L}(\boldsymbol{x}) : (\varepsilon(\boldsymbol{u}^*(\boldsymbol{x})) + \overline{\varepsilon}) + \boldsymbol{L}^0 : \overline{\varepsilon}, \quad \boldsymbol{\delta L}(\boldsymbol{x}) \; = \; \boldsymbol{L}(\boldsymbol{x}) - \boldsymbol{L}^0.$$

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Use solution of the auxiliary problem :

$$\boldsymbol{\varepsilon}(\boldsymbol{u}^*) = -\boldsymbol{\Gamma}^0 * \boldsymbol{\tau} = -\boldsymbol{\Gamma}^0 * (\boldsymbol{\delta L} : \boldsymbol{\varepsilon}(\boldsymbol{u})) - \boldsymbol{\Gamma}^0 * (\boldsymbol{L}^0 : \overline{\boldsymbol{\varepsilon}}) = -\boldsymbol{\Gamma}^0 * (\boldsymbol{\delta L} : \boldsymbol{\varepsilon}(\boldsymbol{u})) \, .$$

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \boldsymbol{\varepsilon}(\boldsymbol{u})^* + \overline{\boldsymbol{\varepsilon}} \; \Rightarrow \quad \boxed{\boldsymbol{\varepsilon}(\boldsymbol{u}) = -\boldsymbol{\Gamma}^0 * (\boldsymbol{\delta L} : \boldsymbol{\varepsilon}(\boldsymbol{u})) + \overline{\boldsymbol{\varepsilon}}.}$$

Lippman-Schwinger integral equation

Iterative scheme :

$$\varepsilon(\boldsymbol{u}^{i+1}) = -\boldsymbol{\Gamma}^0 * \left(\boldsymbol{\delta L} : \varepsilon(\boldsymbol{u}^i)\right) + \overline{\varepsilon}.$$

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Using the properties of the Green operator $\boldsymbol{\Gamma}^0$

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$$\boxed{\varepsilon(\boldsymbol{u}^{\mathsf{i}+1}) = \varepsilon(\boldsymbol{u}^{\mathsf{i}}) - \boldsymbol{\Gamma}^0 * (\boldsymbol{\sigma}^{\mathsf{i}}), \quad \boldsymbol{\sigma}^{\mathsf{i}} = \boldsymbol{L} : \varepsilon(\boldsymbol{u}^{\mathsf{i}}).}$$

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$$\boxed{\varepsilon(\boldsymbol{u}^{i+1}) = \varepsilon(\boldsymbol{u}^i) - \boldsymbol{\Gamma}^0 * (\boldsymbol{\sigma}^i), \quad \boldsymbol{\sigma}^i = \boldsymbol{L} : \varepsilon(\boldsymbol{u}^i).}$$

Alternatively :

$$\boxed{\underbrace{\boldsymbol{\sigma}^i = \boldsymbol{L} : \varepsilon(\boldsymbol{u}^i) \text{ in real space}}_{\text{Constitutive relations}} \quad , \quad \underbrace{\hat{\varepsilon}^{i+1}(\boldsymbol{\xi}) = \hat{\varepsilon}^i(\boldsymbol{\xi}) - \hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}^i(\boldsymbol{\xi}) \text{ in Fourier space}}_{\text{Compatibility and equilibrium}}.}$$

Nonlinear constitutive relations

$$\boldsymbol{\sigma} = \mathcal{F}\left(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{u})\right),$$

re-written as $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}^0 : \boldsymbol{\varepsilon}(\boldsymbol{u}^*(\boldsymbol{x})) \; + \; \boldsymbol{\tau}(\boldsymbol{x})$,

$$\boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{\delta\mathcal{F}}(\boldsymbol{x}), \boldsymbol{\varepsilon}) + \boldsymbol{L}^0 : \overline{\boldsymbol{\varepsilon}}, \quad \boldsymbol{\delta\mathcal{F}}(\boldsymbol{x}, \boldsymbol{\varepsilon}) \; = \; \boldsymbol{\mathcal{F}}(\boldsymbol{x}, \boldsymbol{\varepsilon}) - \boldsymbol{L}^0 : \boldsymbol{\varepsilon}.$$

Nonlinear constitutive relations

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Nonlinear integral Lipmann-Schwinger equation :

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = -\boldsymbol{\Gamma}^0 * \boldsymbol{\delta\mathcal{F}}\left(\boldsymbol{\varepsilon}(\boldsymbol{u})\right) + \bar{\boldsymbol{\varepsilon}}.$$

Nonlinear constitutive relations

$$\boldsymbol{\sigma} = \mathcal{F}\left(x, \varepsilon(u)\right),$$

re-written as $\boldsymbol{\sigma}(x) = \boldsymbol{L}^0 : \varepsilon(u^*(x)) \; + \; \boldsymbol{\tau}(x)$,

$$\boldsymbol{\tau}(x) = \boldsymbol{\delta\mathcal{F}}(x), \varepsilon) + \boldsymbol{L}^0 : \overline{\varepsilon}, \quad \boldsymbol{\delta\mathcal{F}}(x, \varepsilon) \; = \; \boldsymbol{\mathcal{F}}(x, \varepsilon) - \boldsymbol{L}^0 : \varepsilon.$$

Nonlinear integral Lipmann-Schwinger equation :

$$\boxed{\varepsilon(u) = -\Gamma^0 * \boldsymbol{\delta\mathcal{F}}\left(\varepsilon(u)\right) + \overline{\varepsilon}.}$$

Iterative scheme

$$\varepsilon(u^{i+1}) = -\Gamma^0 * \boldsymbol{\delta\mathcal{F}}\left(\varepsilon(u^i)\right) + \overline{\varepsilon} = \varepsilon(u^i) - \Gamma^0 * \boldsymbol{\mathcal{F}}\left(\varepsilon(u^i)\right) = \varepsilon(u^i) - \Gamma^0 * \boldsymbol{\sigma}^i.$$

$\boldsymbol{\sigma}^i = \mathcal{F}\left(\varepsilon(u^i)\right)$ in real space, $\quad \hat{\varepsilon}^{i+1}(\boldsymbol{\xi}) = \hat{\varepsilon}^i(\boldsymbol{\xi}) - \hat{\Gamma}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}^i(\boldsymbol{\xi})$ in Fourier space.

Algorithm

Initialization : $\boldsymbol{\varepsilon}^0(\boldsymbol{x}) = \overline{\boldsymbol{\varepsilon}},\ \boldsymbol{\sigma}^0(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{\varepsilon}^0(\boldsymbol{x}),\ \forall\, \boldsymbol{x} \in\ V,$

Iterate i+1 : ε^{i} and $\boldsymbol{\sigma}^{\mathsf{i}}$ being known, do untill convergence :

Real space		**Fourier space**
$\boldsymbol{\sigma}^{\mathsf{i}}$	$\overset{FFT}{\rightarrow}$	$\hat{\boldsymbol{\sigma}}^{\mathsf{i}}$
		$\hat{\boldsymbol{\varepsilon}}^{\mathsf{i}+1}(\boldsymbol{\xi}) = \hat{\boldsymbol{\varepsilon}}^{\mathsf{i}}(\boldsymbol{\xi}) - \hat{\boldsymbol{\Gamma}}^0(\boldsymbol{\xi}) : \hat{\boldsymbol{\sigma}}^{\mathsf{i}}(\boldsymbol{\xi})$
		$\hat{\boldsymbol{\varepsilon}}^{\mathsf{i}+1}(0) = \overline{\boldsymbol{\varepsilon}}$
$\boldsymbol{\varepsilon}^{\mathsf{i}+1}(\boldsymbol{x})$	$\overset{(FFT)^{-1}}{\leftarrow}$	$\hat{\boldsymbol{\varepsilon}}^{\mathsf{i}+1}(\boldsymbol{\xi})$
$\boldsymbol{\sigma}^{\mathsf{i}+1}(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{\varepsilon}^{\mathsf{i}+1}(\boldsymbol{x})$		

Algorithm

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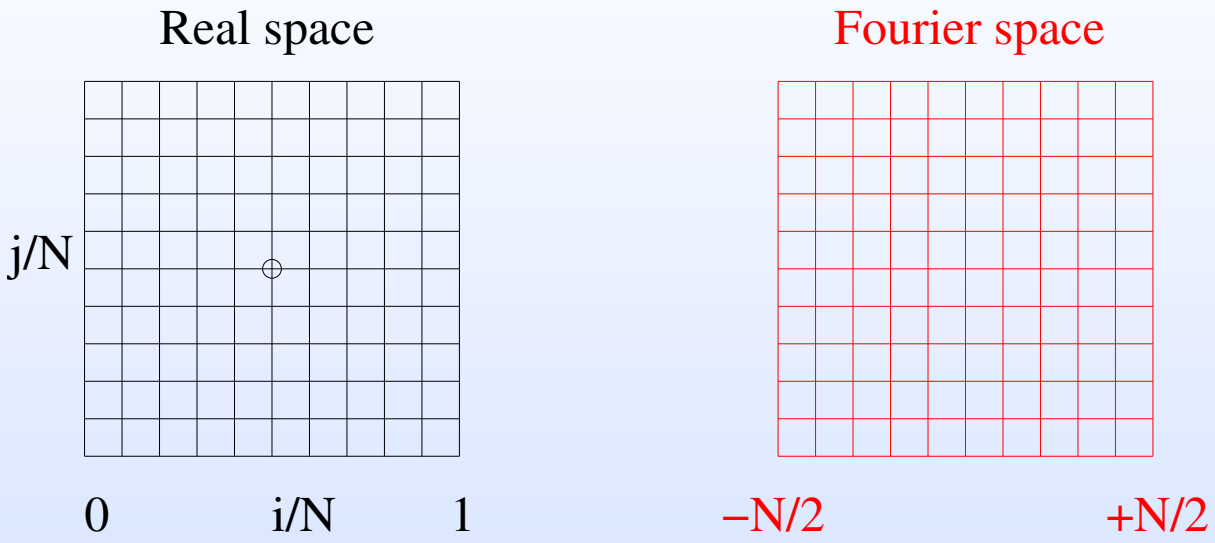
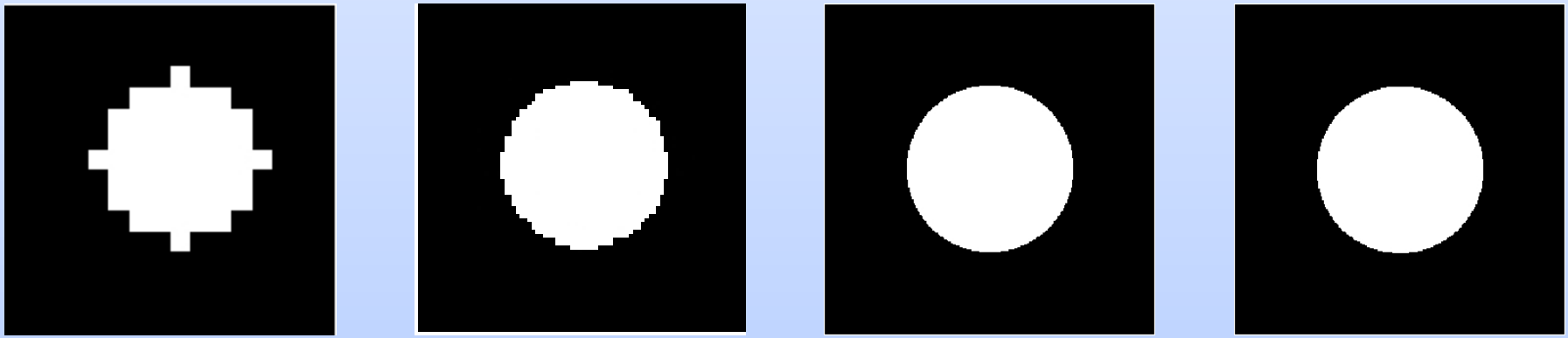
$\boldsymbol{\varepsilon}^{\mathrm{i}+1}(\boldsymbol{x})$	$\overset{(FFT)^{-1}}{\leftarrow}$	$\hat{\boldsymbol{\varepsilon}}^{\mathrm{i}+1}(\boldsymbol{\xi})$
$\boldsymbol{\sigma}^{\mathrm{i}+1}(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{\varepsilon}^{\mathrm{i}+1}(\boldsymbol{x})$		

- Constitutive relations are **“local”** in real space : $\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{x})$ can be computed independently at each $\boldsymbol{x}$.

- Equilibrium and compatibility equations are **“nonlocal”** in real space, but are **local in Fourier space**.

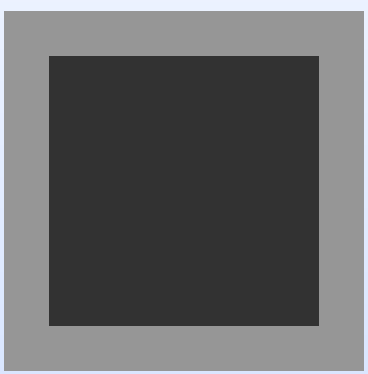


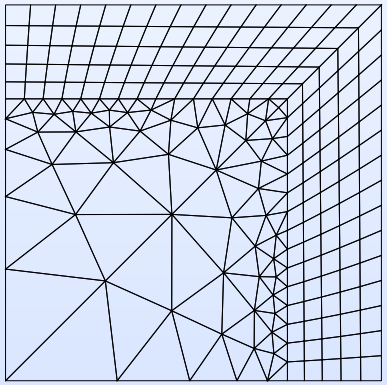
Spatial resolution = **Number of pixels or voxels in the image**.

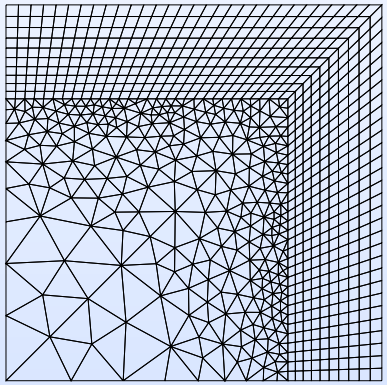


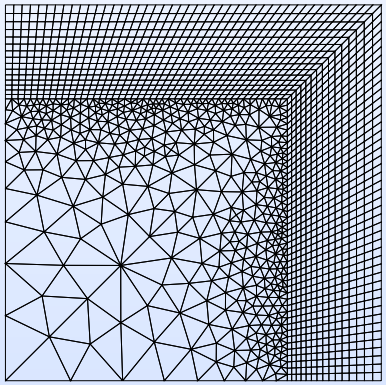
16 × 16 64 × 64 256 × 256 1024 × 1024

Comparison FFT/FEM 2 elastic plastic phases $\sigma_0^m = 100$ Mpa, $\sigma_0^f = 500$ Mpa.

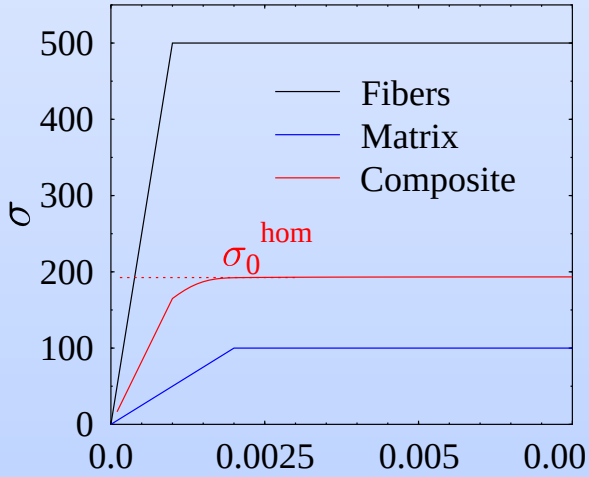








Resol. N	FFT σ_0^{hom} MPa	FFT CPU time s	Dof's	FEM σ_0^{hom} MPa	FEM CPU time s
16	160.34	1.64	*	*	*
32	160.66	3.02	1402	162.36	267.69
64	**160.07**	**12.21**	**5710**	**160.62**	**2170.28**
128	159.55	53.53	11370	160.37	6464.47
256	159.29	253.31	*	*	*
512	159.13	1075.60	*	*	*



Comments

- **Easy to implement on parallel computers** : constitutive relations in real space, Green's operator in Fourier space.

- **Can be extended to nonlinear behaviors** : incremental plasticity, viscoplasticity, hyperelasticity and finite strains.

- **Faster** than the Finite Element Method.

Comments

- **Easy to implement on parallel computers** : constitutive relations in real space, Green's operator in Fourier space.

- **Can be extended to nonlinear behaviors** : incremental plasticity, viscoplasticity, hyperelasticity and finite strains.

- **Faster** than the Finite Element Method.

- **Limitation** : Rate of convergence $\simeq$ contrast between the phases

$$\varepsilon(\boldsymbol{u}^{i+1}) = -\Gamma^0 * \left(\boldsymbol{\delta L} : \varepsilon(\boldsymbol{u}^{i})\right) + \overline{\varepsilon}.$$

Does not converge for rigidly-reinforced or voided materials.

- Accelerated scheme (Eyre and Milton, 1999) : rate of convergence $\simeq \sqrt{\text{contrast}}$. Convergence still not ensured for composites with infinite contrast.

- Composites with infinite contrast (and power law materials) handled by a different formulation based on **augmented Lagrangians** (Michel, Moulinec & PS, 2001).

3. Accuracy of theoretical estimates for linear composites

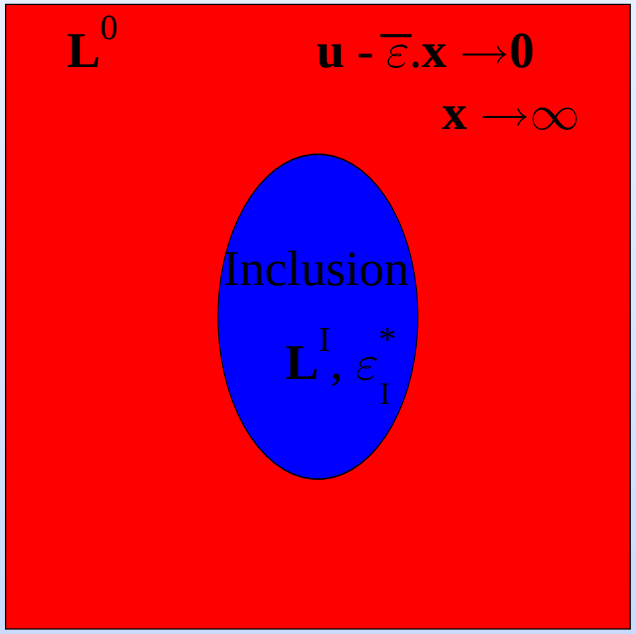
In linear composites, it is sufficient to determine the first moment (average) of the strain over each phase to determine the homogenized constitutive relations.

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{L}^{(r)} : \boldsymbol{\varepsilon}(\boldsymbol{x}) \quad \text{in phase } r, \quad \overline{\boldsymbol{\varepsilon}}_r = \boldsymbol{A}_r : \overline{\boldsymbol{\varepsilon}},$$

$$\overline{\boldsymbol{\sigma}} = \sum_{r=1}^{N} c^{(r)} \overline{\boldsymbol{\sigma}}_r = \sum_{r=1}^{N} c^{(r)} \boldsymbol{L}^{(r)} : \overline{\boldsymbol{\varepsilon}}_r \quad \Rightarrow \quad \overline{\boldsymbol{\sigma}} = \left(\sum_{r=1}^{N} c^{(r)} \boldsymbol{L}^{(r)} : \boldsymbol{A}_r \right) : \overline{\boldsymbol{\varepsilon}}.$$

There is NO need to resolve the local stress and strain fields. It suffices to determine their average per phase.

Classical treatment for linearly elastic constituents



Inclusion problems (Eshelby, 1957) :

elastic ellipsoidal particle in a linear elastic infinite medium subjected to an **average strain** $\overline{\varepsilon}$ at infinity and a **transformation strain** ε_I^*.

- $\boldsymbol{L}^I = \boldsymbol{L}^0$: the strain field is **uniform** in the inclusion :

$$\varepsilon_I = \boldsymbol{\mathcal{S}}^0 : \varepsilon_I^*$$

- $\boldsymbol{L}^I \neq \boldsymbol{L}^0$, $\varepsilon_I^* = 0$: the strain field is uniform in the inclusion :

$$\varepsilon_I = \left(\boldsymbol{I} + \boldsymbol{\mathcal{S}}^0 : (\boldsymbol{L}^0)^{-1} : (\boldsymbol{L}^I - \boldsymbol{L}^0)\right)^{-1} : \overline{\varepsilon}$$

In both problems, **the strain field is uniform in the inclusion phase.**

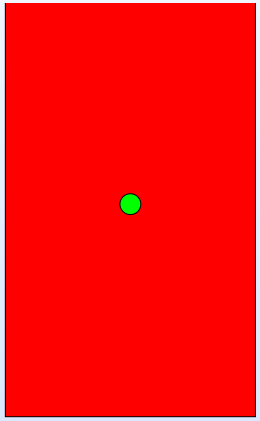
Most linear schemes derive from Eshelby's result :

- **Inclusion-matrix systems** :

Dilute approximation

$\boldsymbol{L}^0 = \boldsymbol{L}^{\text{matrix}}$, $\boldsymbol{\varepsilon}_I^* = 0$.

No interaction between inclusions accounted for : valid for small concentrations.



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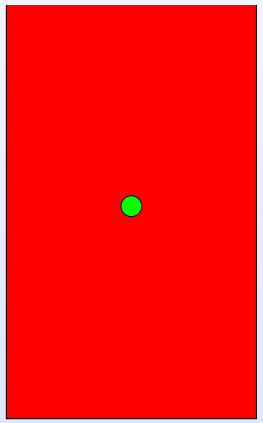
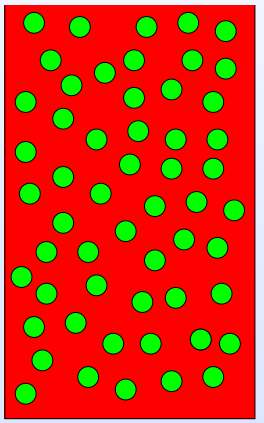


Hashin-Shtrikman bounds

$\boldsymbol{L}^0 = \boldsymbol{L}^{\text{opt}}$, $\boldsymbol{\varepsilon}_I^*$ uniform.

Optimal values of $\boldsymbol{L}^0, \boldsymbol{\varepsilon}_I^*$ determined through variational principles.



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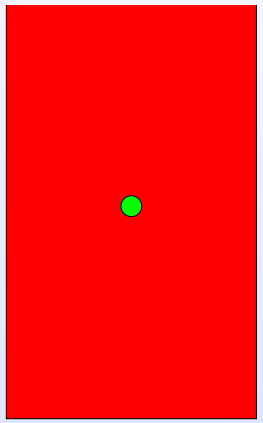

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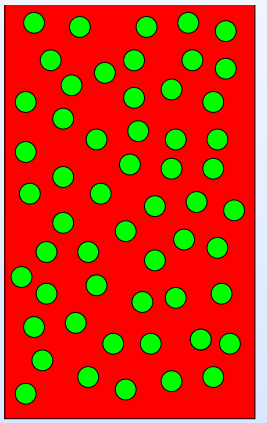
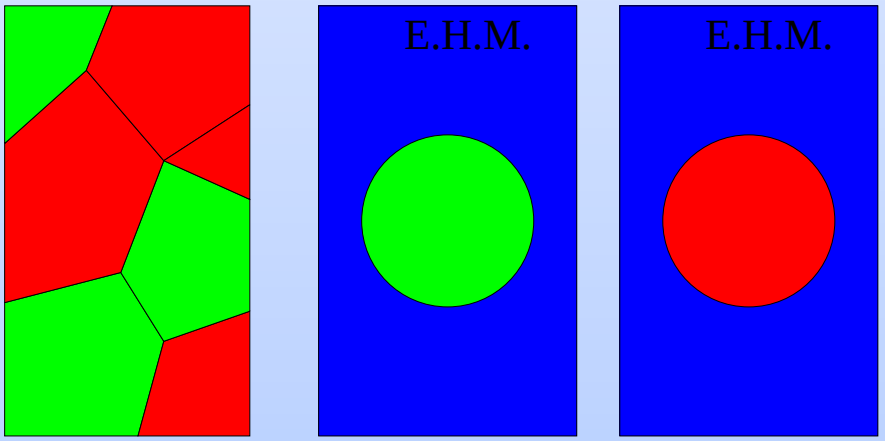


- **Polycrystals :**

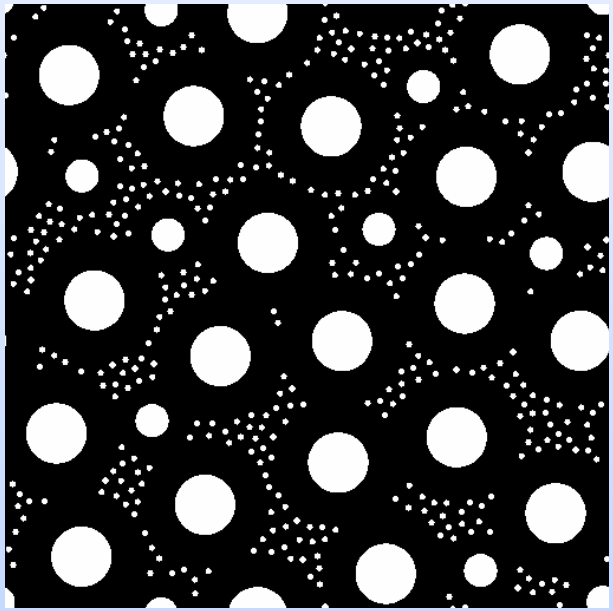
No phase plays the role of a matrix.
Self-consistent scheme (Budiansky, Kröner, Hill) :
reference medium = equivalent homogeneous medium.



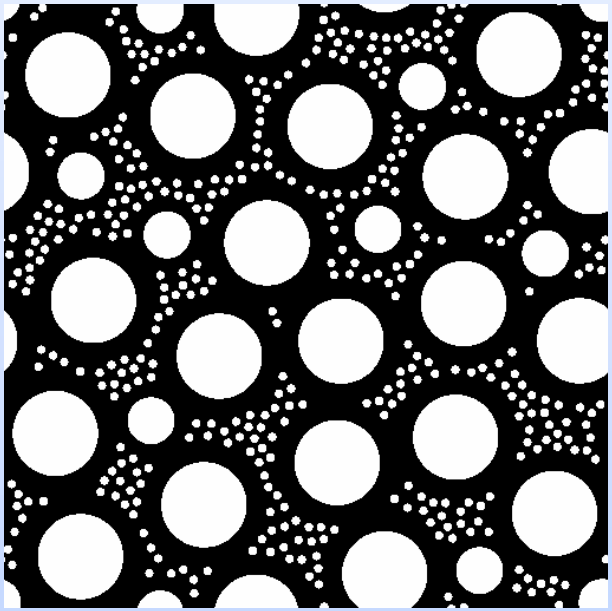
The self-consistent approximation assumes that the strain is uniform in the grains.

Two-phase inclusion-matrix composites

Two-phase composite cylinders assemblage with three different fiber sizes. **Idea :** microstructures for which one of the Hashin-Shtrikman bound is attained (isotropic phases).



$c^{(1)} = 0.2105$

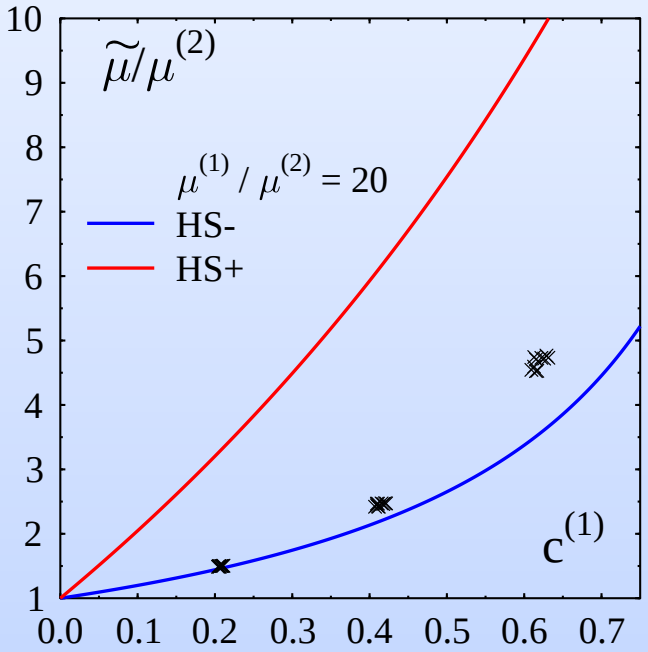


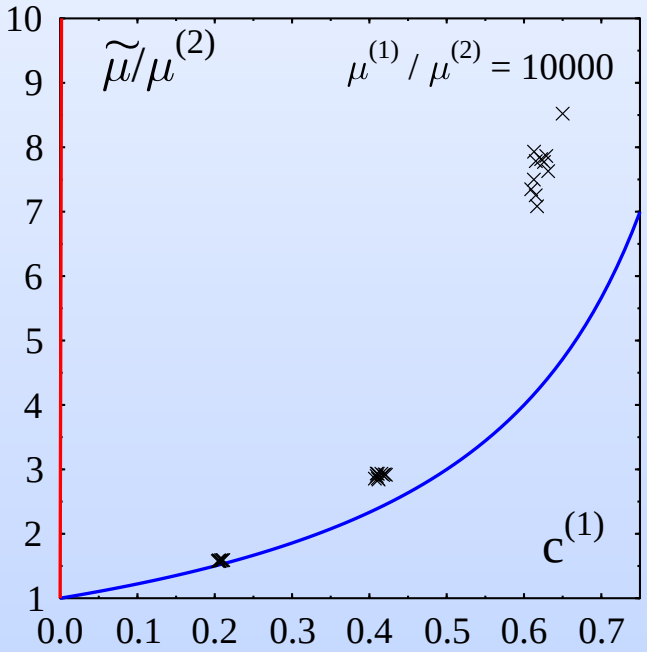
$c^{(1)} = 0.4209$

20 realizations for “ideal” fiber volume fraction : 0.25, 0.5, 0.75. (actual volume fractions are smaller).

Effective properties : linear composites Hashin and Shtrikman bounds :

$$\widetilde{\mu}_{-}^{\mathrm{HS}} = \mu^{(2)} + c^{(1)} \frac{\mu^{(1)} - \mu^{(2)}}{1 + c^{(2)} \dfrac{2(\mu^{(1)} - \mu^{(2)})}{(2+d)\mu^{(2)}}}, \qquad \widetilde{\mu}_{+}^{\mathrm{HS}} \ : \text{ interchange } \mu^{(1)} \text{ and } \mu^{(2)}.$$

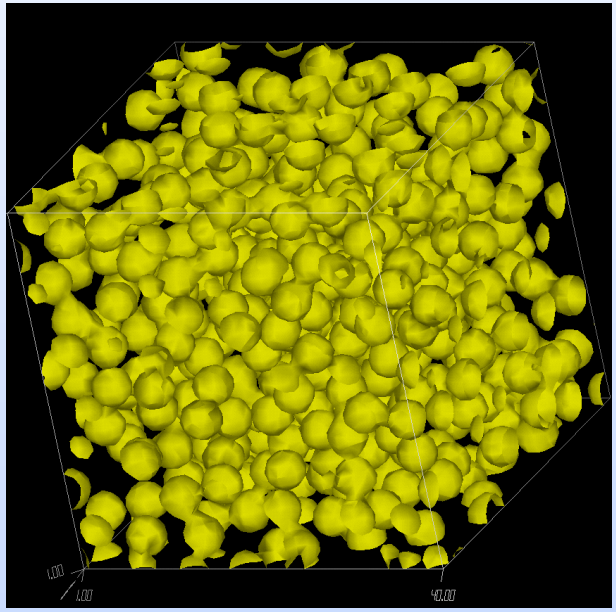


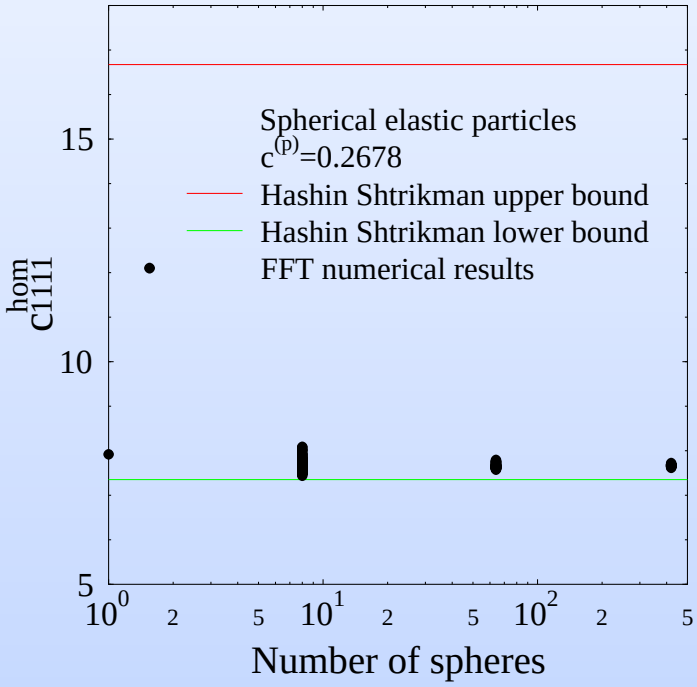


Why such a high contrast ? : Nonlinear composites $\simeq$ linear composites with high contrast. **Satisfactory agreement satisfactory with HS- bound when** $c^{(1)} \leq 0.5$**.**

Elastic properties of 3d particle-matrix composites.

Suspension of monodisperse spherical inclusions in an elastic matrix.

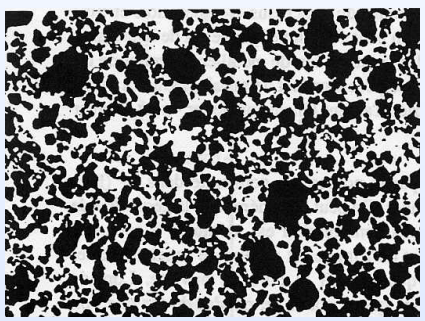
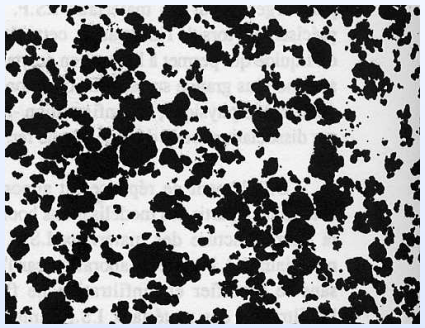
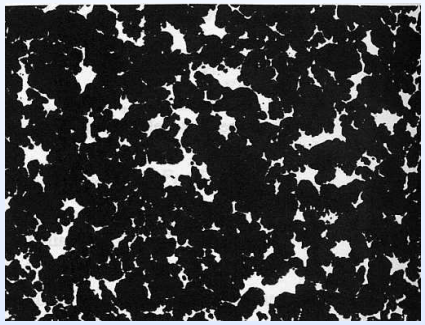
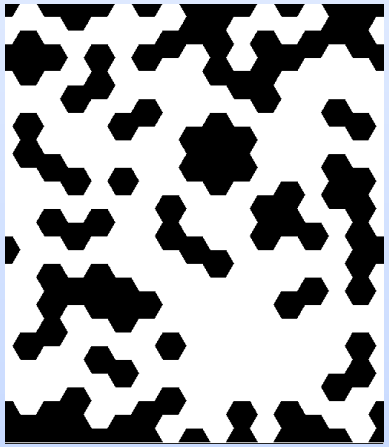
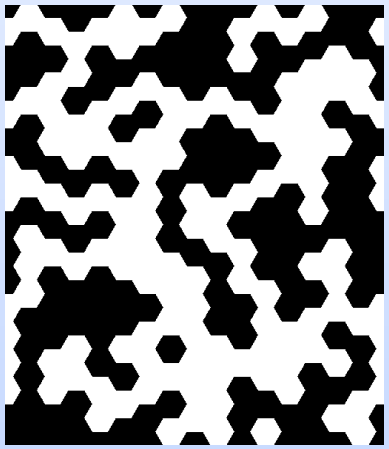
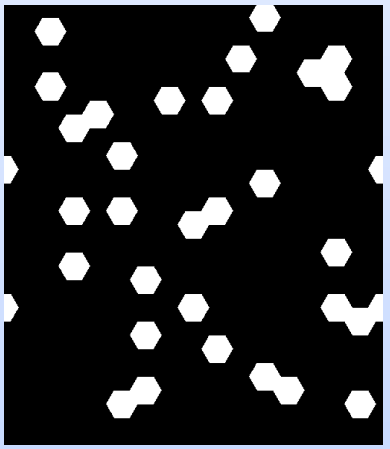




Elastic properties

Number of particles	Number of tests	$\widetilde{L}_{1111}$ mean (GPa)	$\widetilde{L}_{1111}$ std deviation
1	1	7.919	-
8	101	7.675	0.142
64	40	7.664	0.054
420	21	7.667	0.024

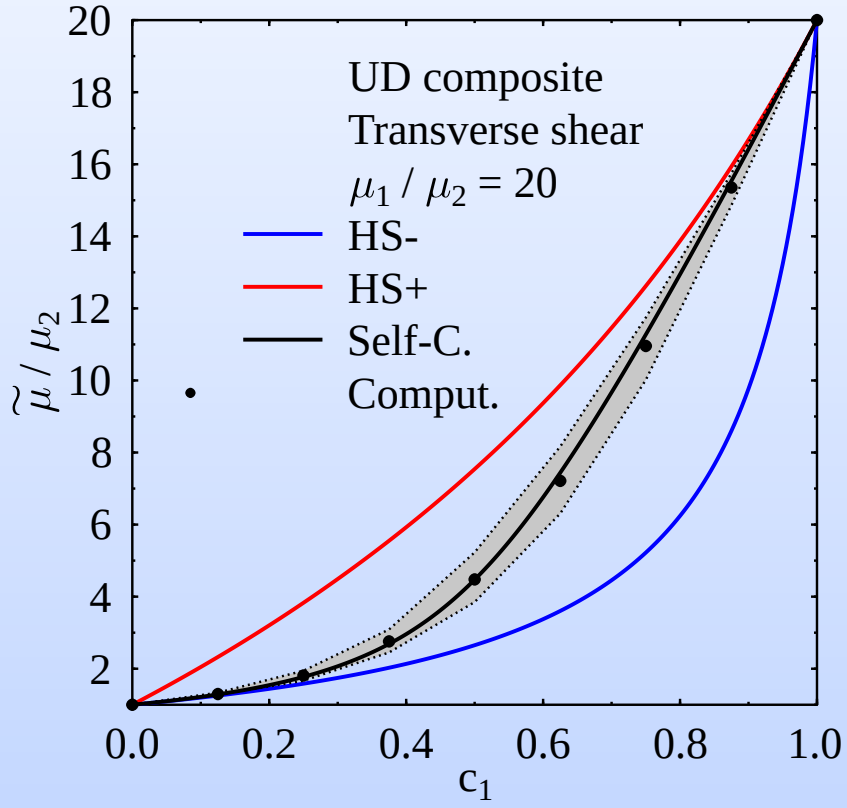
Two-phase, Granular type of microstructures

Covering by identical hexagons. Properties of the hexagons chosen randomly (phase 1 or phase 2). 200 different configurations for each volume fraction.

Contiguity of the phases : depends on the volume fraction. Inclusion / matrix type of microstructure at low and high volume fraction.

Transverse shear modulus



200 configurations

Hashin Shtrikman bounds :

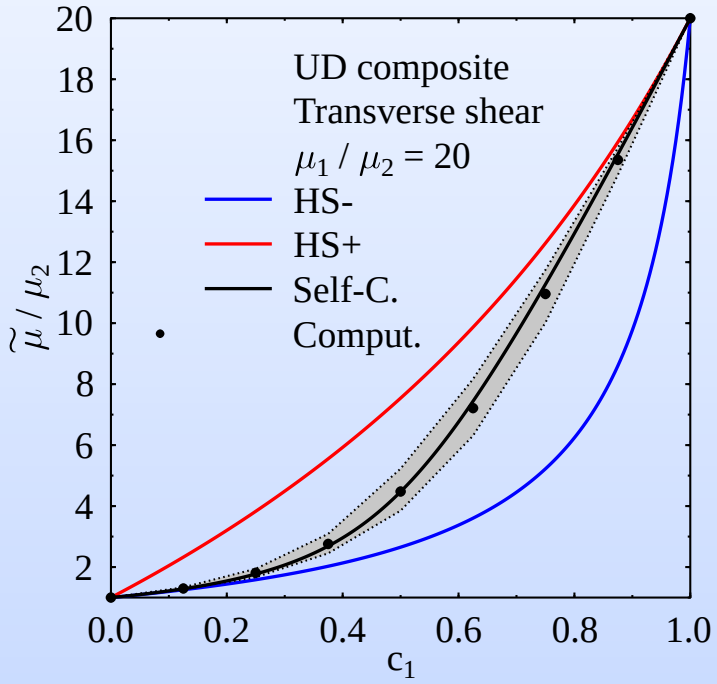
$$\mu^{HS-} = \mu^{(2)} + c^{(1)} \frac{\mu^{(1)} - \mu^{(2)}}{1 + c^{(2)} \frac{\mu^{(1)} - \mu^{(2)}}{2\mu^{(2)}}},$$

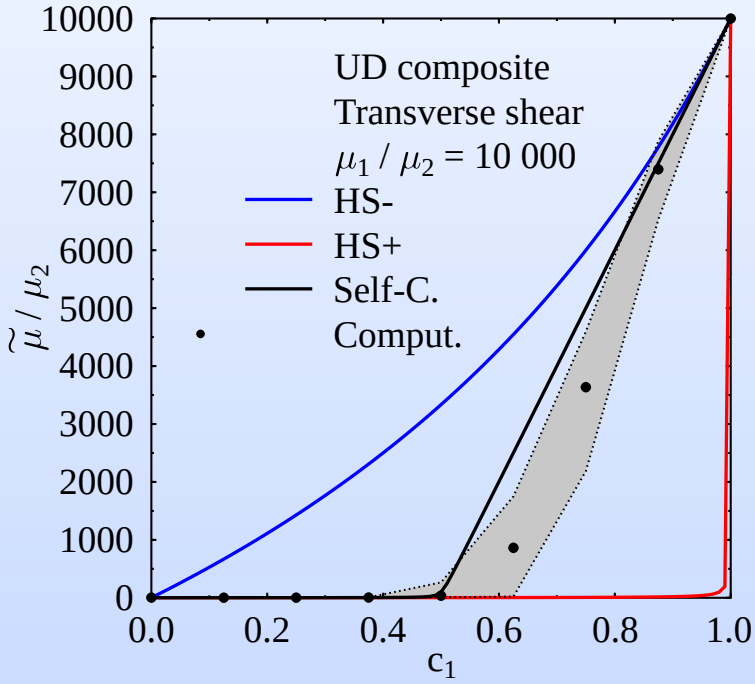
$$\mu^{HS+} = \mu^{(2)} + c^{(1)} \frac{\mu^{(1)} - \mu^{(2)}}{1 + c^{(2)} \frac{\mu^{(1)} - \mu^{(2)}}{\mu^{(1)} + \mu^{(2)}}}$$

Self-consistent scheme :

$$\mu^{SC} = \frac{1}{2} \Big((c^{(1)} - c^{(2)})(\mu^{(1)} - \mu^{(2)}) + \sqrt{(c^{(2)} - c^{(1)})^2 (\mu^{(2)} - \mu^{(1)})^2 + 4\mu^{(1)}\mu^{(2)}} \Big)$$

Not accurate at all contrast



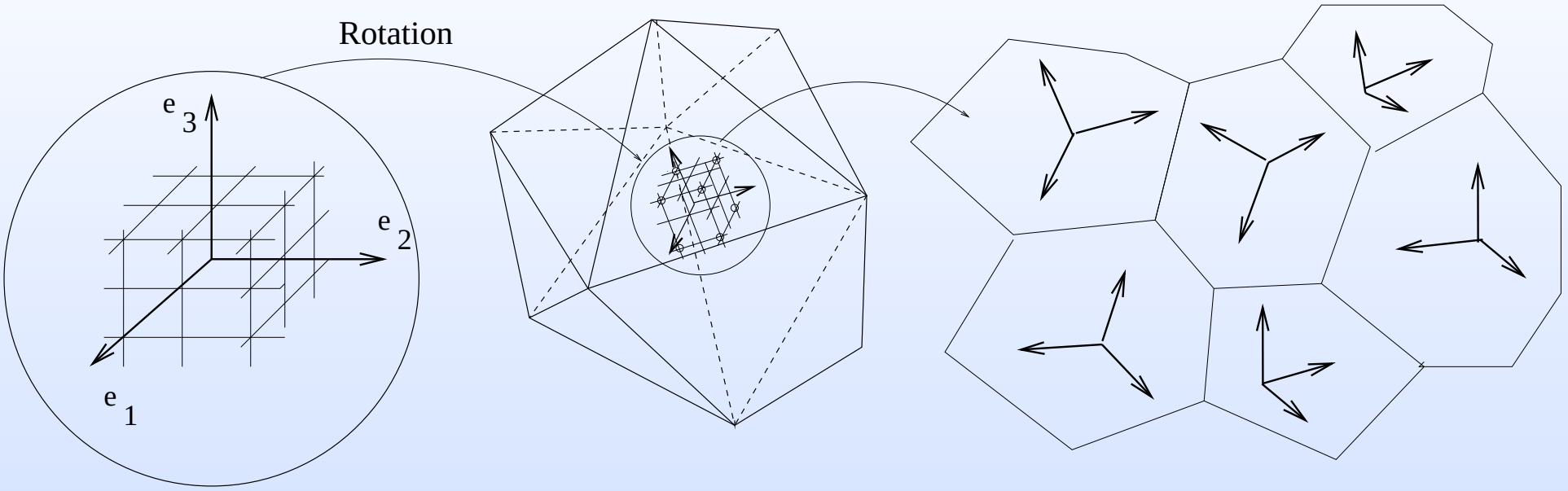


contrast=20

contrast=10^4.

Percolation threshold : correct. **Percolation exponent** : not correct.

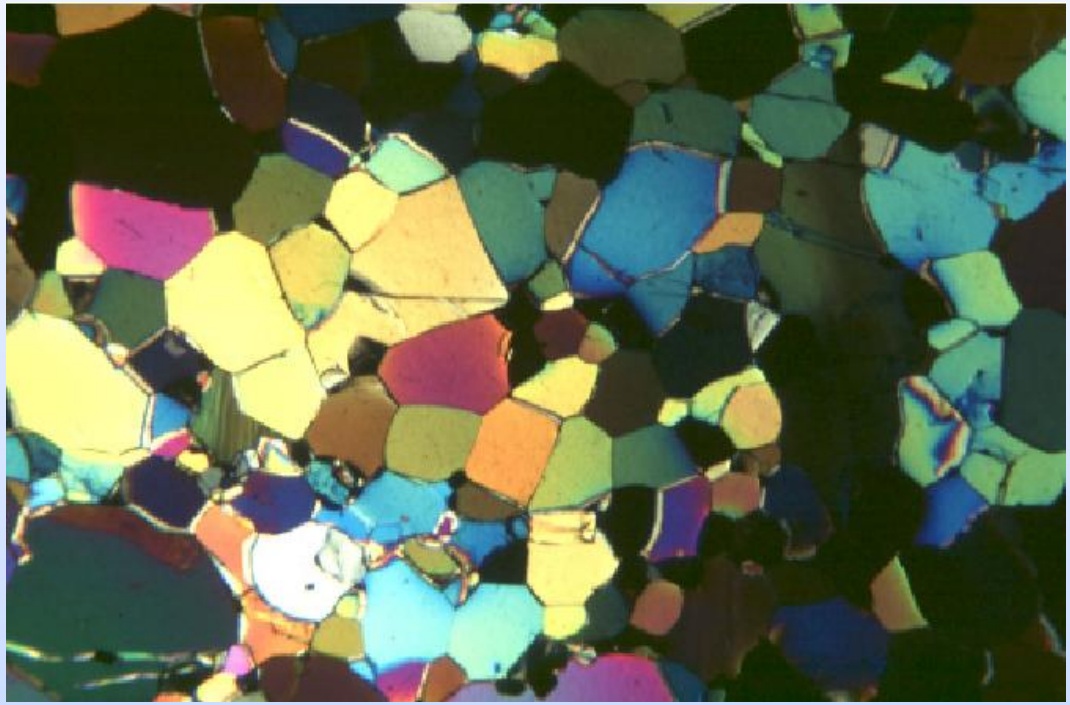
Polycrystals



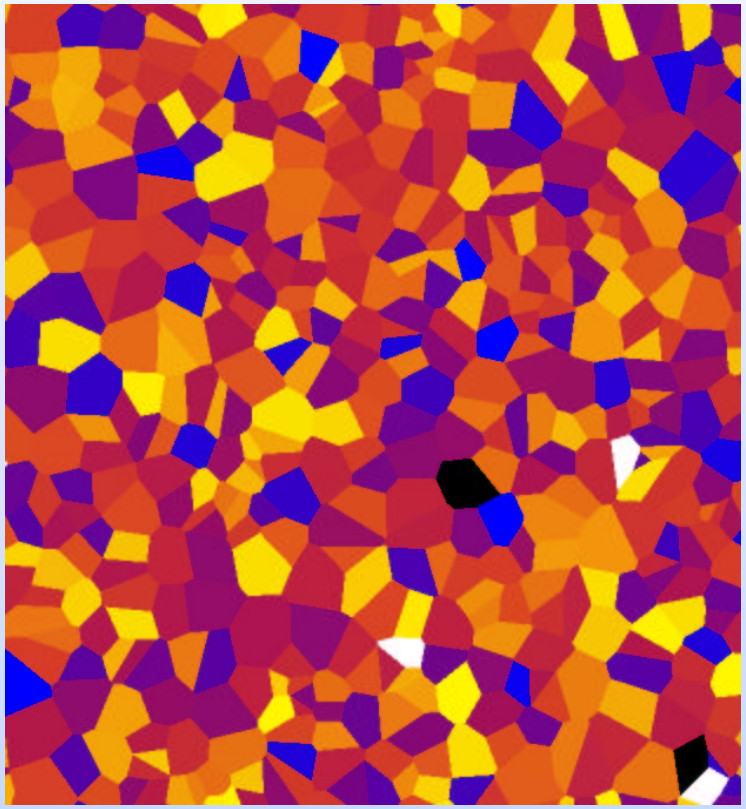
Each grain is a copy of the same single crystal, except for its orientation θ which varies from grain to grain.

- **Stiffness for the single crystal L^s.**
- **Stiffness for a rotated grain $L^s_{\theta(x)} = {}^{\mathsf{T}}R.{}^{\mathsf{T}}R.L^s.R.R.$**
- **Effective stiffness for the polycrystal (aggregate of grains) :**

$$\frac{1}{2}\overline{\varepsilon} : \boldsymbol{L}^p : \overline{\varepsilon} = \inf_{\boldsymbol{u}\in\mathcal{K}(\overline{\varepsilon})} \frac{1}{2} < \varepsilon(\boldsymbol{u})) : \boldsymbol{L}^s_{\theta(\boldsymbol{x})} : \varepsilon(\boldsymbol{u})) > .$$



Real microstructure
Optical micrograph



Simulated microstructure
Voronoi tesselation : 512 grains.

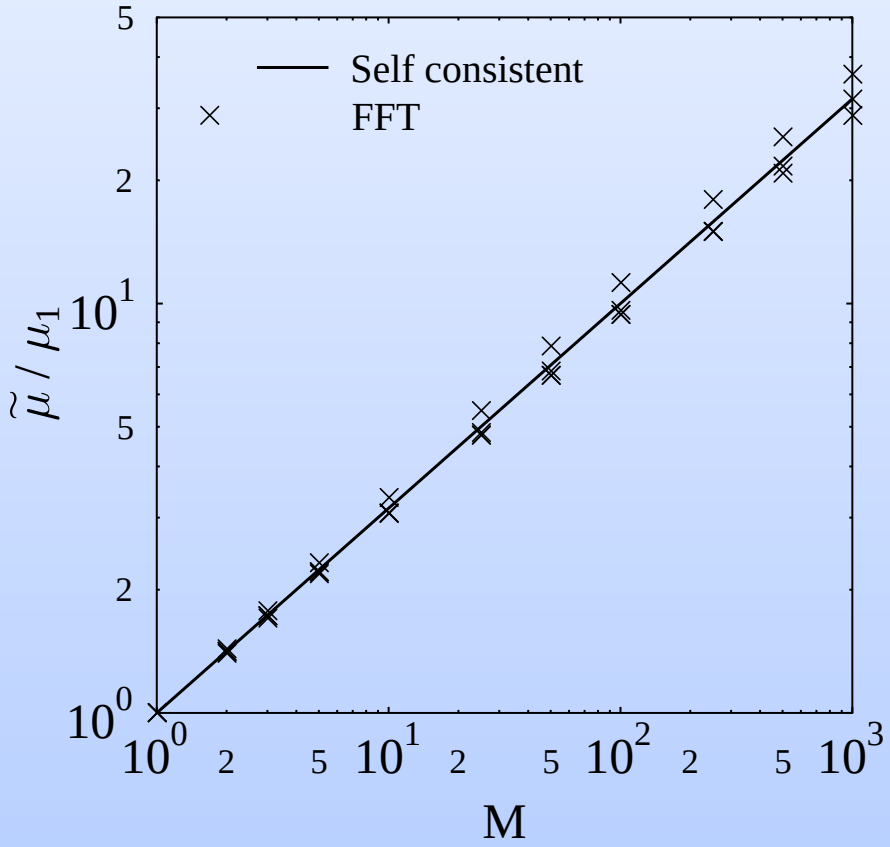
Antiplane shear-modulus

$$\sigma_{13} = 2\mu_1\varepsilon_{13},\ \sigma_{23} = 2\mu_2\varepsilon_{23}, \quad M = \mu_1/\mu_2$$

Self-consistent scheme :

$$\tilde{\mu} = \sqrt{M}\mu^{(2)}.$$

Agrement is good even at high contrast.



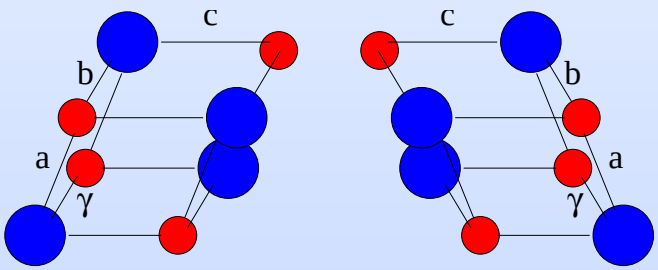
Comments

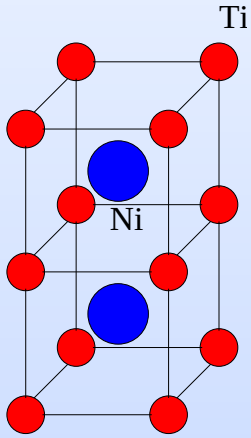
- **At moderate contrast :** Effective properties of common microstructures are accurately described by the Hashin-Shtrikman bounds or self-consistent scheme.
- **Inclusion-matrix morphology :** Hashin-Shtrikman bounds.
- **“Granular” morphology :** self-consistent.

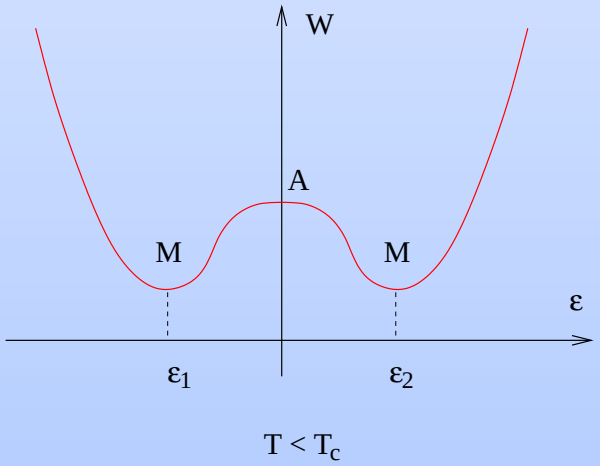
4. A case study for nonlinear composites

Recoverable strains in polycrystals

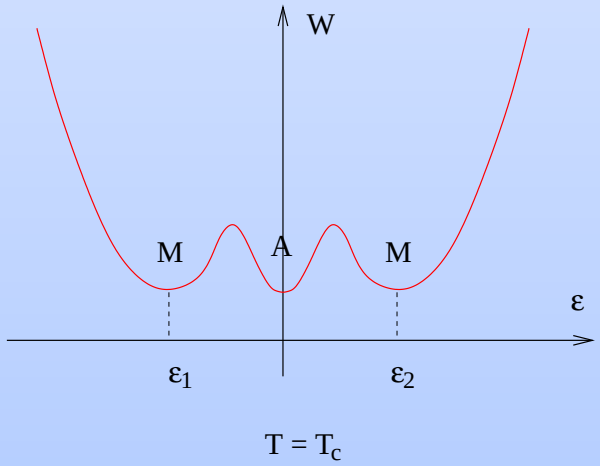
Shape memory effect in single crystals by martensitic transformation = change in lattice symmetry :



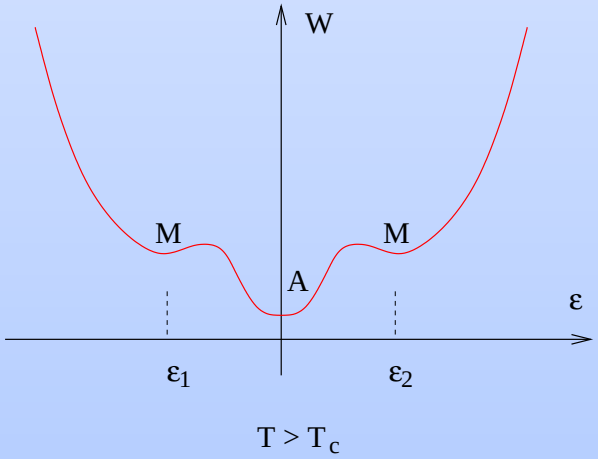




T < T_c



T = T_c



T > T_c

Relaxation and Microstructures in single crystals

Take a volume element V composed of only the **homogeneous material** (single crystal) with energy w. Consider the **variational problem :**

$$\inf_{u \in \mathcal{K}(\overline{\varepsilon})} \langle w(\varepsilon(u)) \rangle, \tag{1}$$

$$\mathcal{K}(\overline{\varepsilon}) = \{\varepsilon = \text{grad}\,(u) \text{ in } V,\ u = \overline{\varepsilon}.\boldsymbol{x} + v,\ v\# \text{ on } \partial V\}.$$

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- Initial energy w **nonconvex**. Although the material is homogeneous, the best minimizer in (1) is **NOT necessarily** $\varepsilon = \overline{\varepsilon}$.
- Minimization problems well-posed with the relaxed (or effective) energy

$$Qw(\overline{\varepsilon}) = \inf_{u \in \mathcal{K}(\overline{\varepsilon})} \langle w(\varepsilon(u)) \rangle.$$

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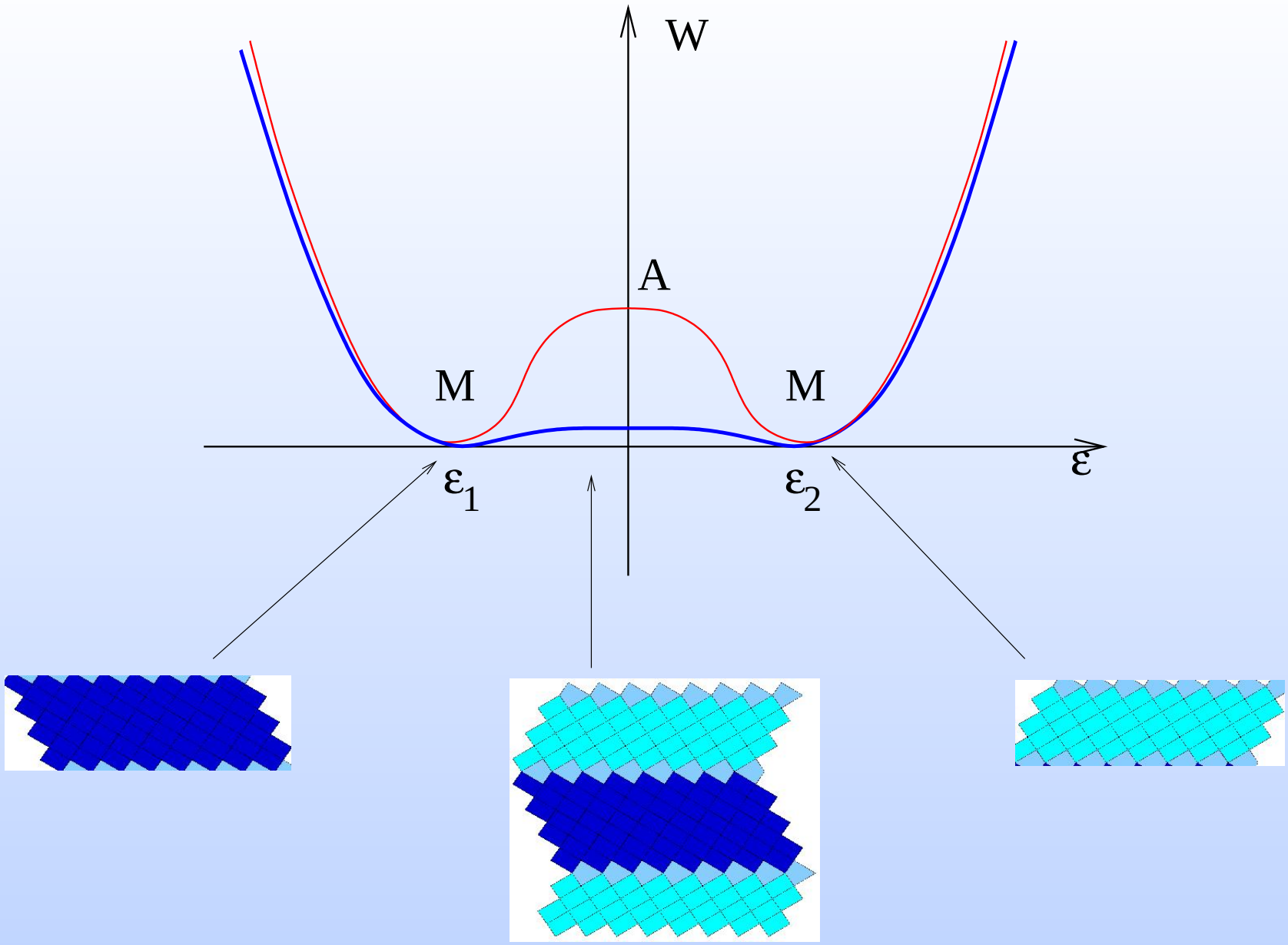
$$Qw(\overline{\varepsilon}) = \inf_{u \in \mathcal{K}(\overline{\varepsilon})} \langle w(\varepsilon(u)) \rangle.$$

- Approximate minimizers (fields $\varepsilon(x)$) are fine mixtures of energy-wells. **Formation of fine microstructures** (Ball and James, 1987).



Note that there is a domain of **low energy** in strain space : **domain of recoverable strains for the single crystal.**

The shape memory effect in polycrystals

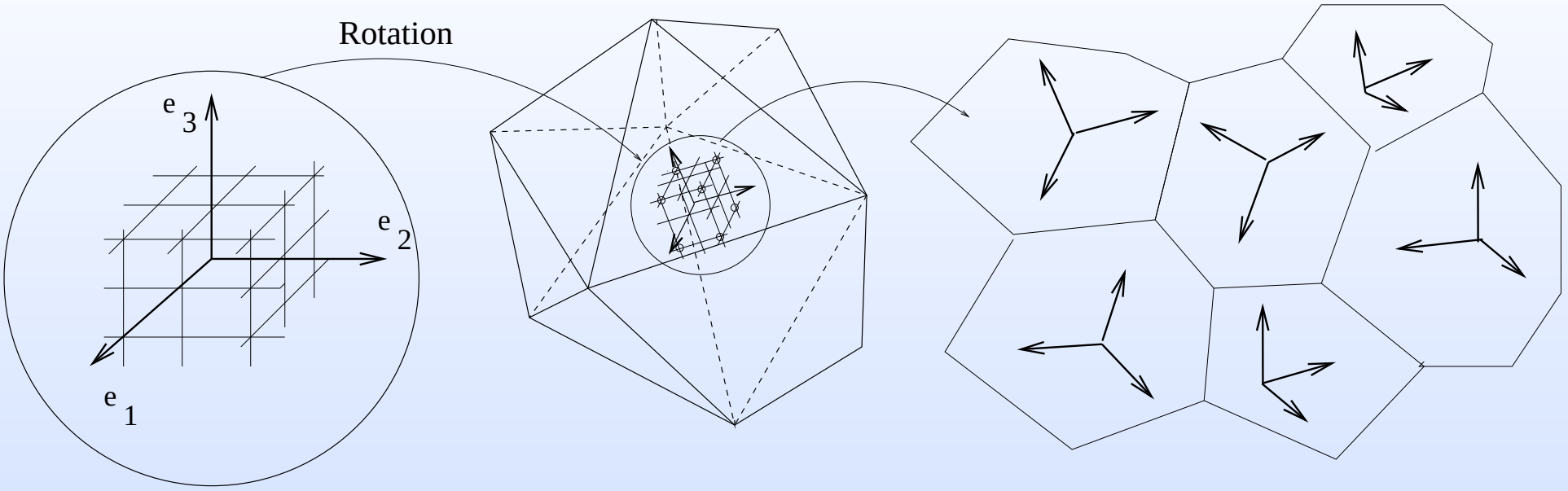
Typical commercial specimens are **polycrystals. Observations :**

- The same material might exhibit **very different shape memory behavior** as a single crystal or as a polycrystal.
- Many materials exhibit good shape memory behavior as single crystals but little or none as polycrystals. Typical figures for recoverable strains :

Alloy	Single crystal	Polycrystal
Ni-Al	0 - 13 %	Negligible
Fe-Ni-C	0 - 12 %	Negligible
Cu-Al-Ni	2 - 9 %	2 % (textured ribbons : 6 %)
Ni-Ti	3 - 10 %	5 - 8 %

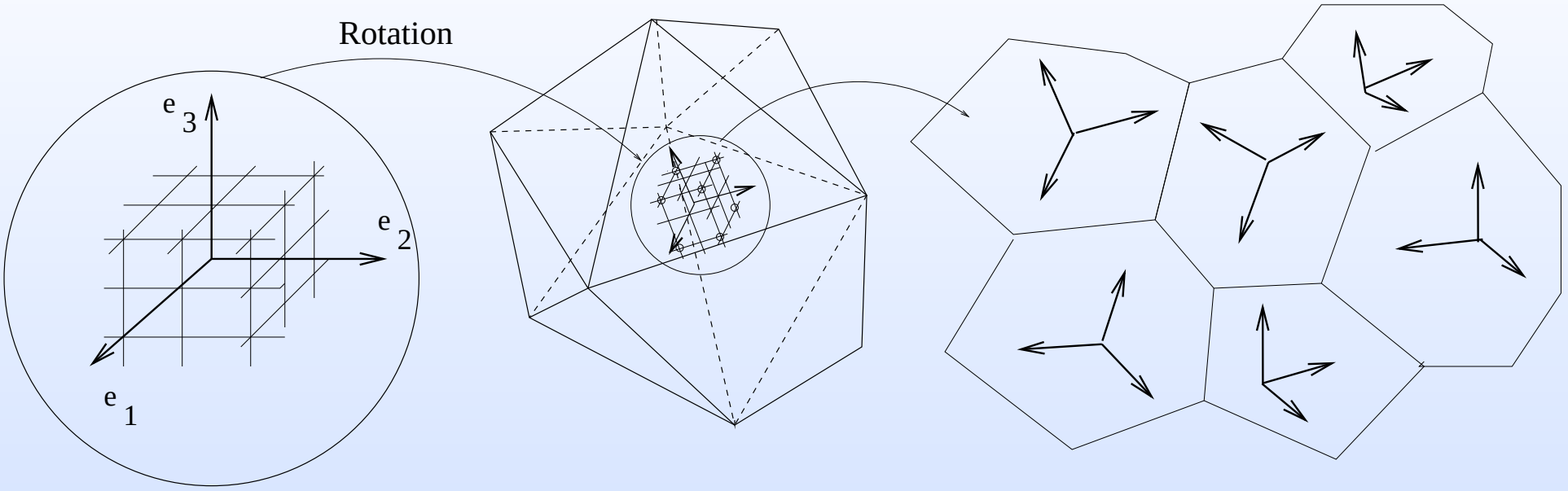
- **Why is there such a difference between single crystals and polycrystals ?**

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



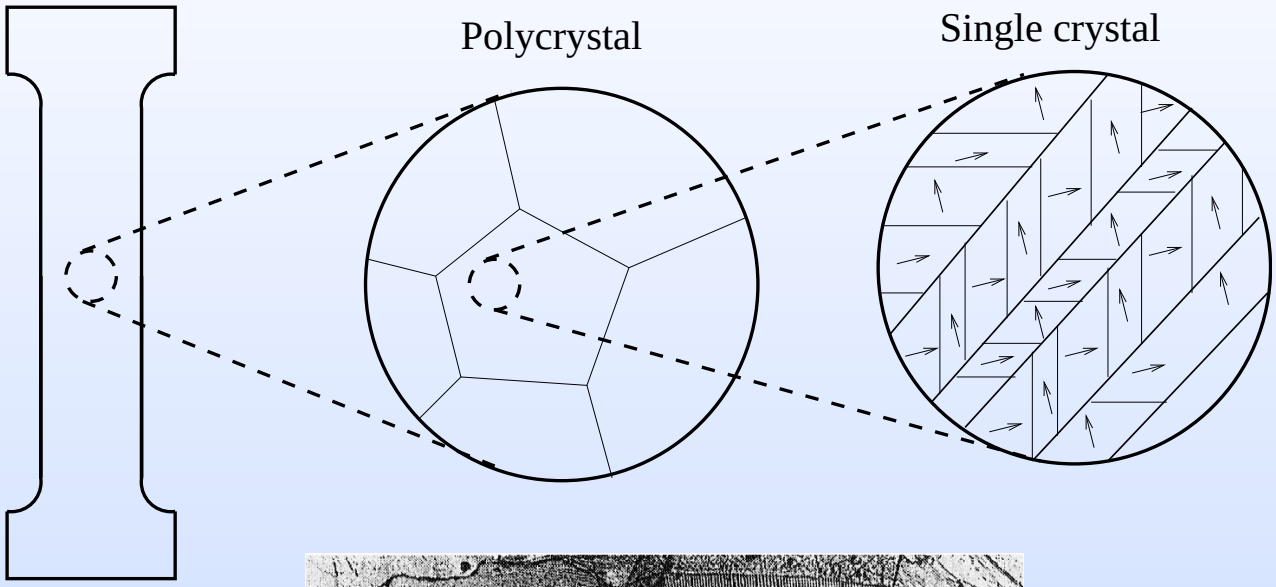
Each grain is a copy of the same single crystal, with energy w^s except for its orientation θ which varies from grain to grain.

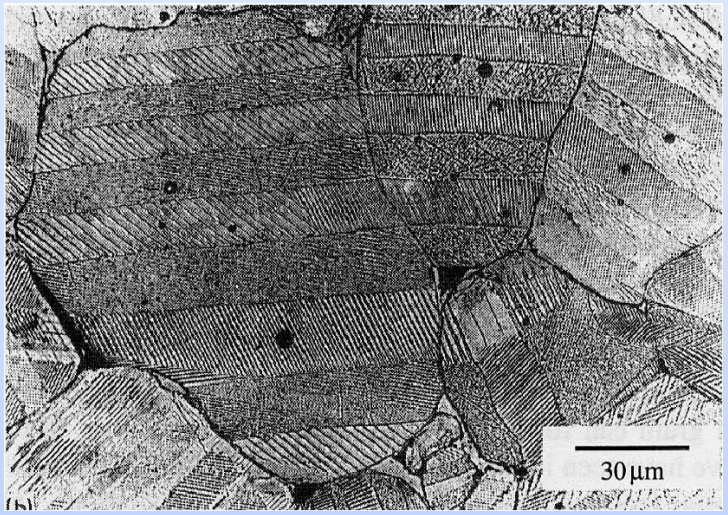
- **Energy for the single crystal $w^s(\varepsilon)$.**
- **Energy for a rotated grain $w^s(\boldsymbol{R}, \varepsilon)$.**
- **Effective energy for the polycrystal (aggregate of grains) :**

$$w^p(\overline{\varepsilon}) = \inf_{\boldsymbol{u} \in \mathcal{K}(\overline{\varepsilon})} < w^s(\boldsymbol{R}(\boldsymbol{x}), \varepsilon(\boldsymbol{u})) > .$$

Homogenization problem for a nonconvex energy.

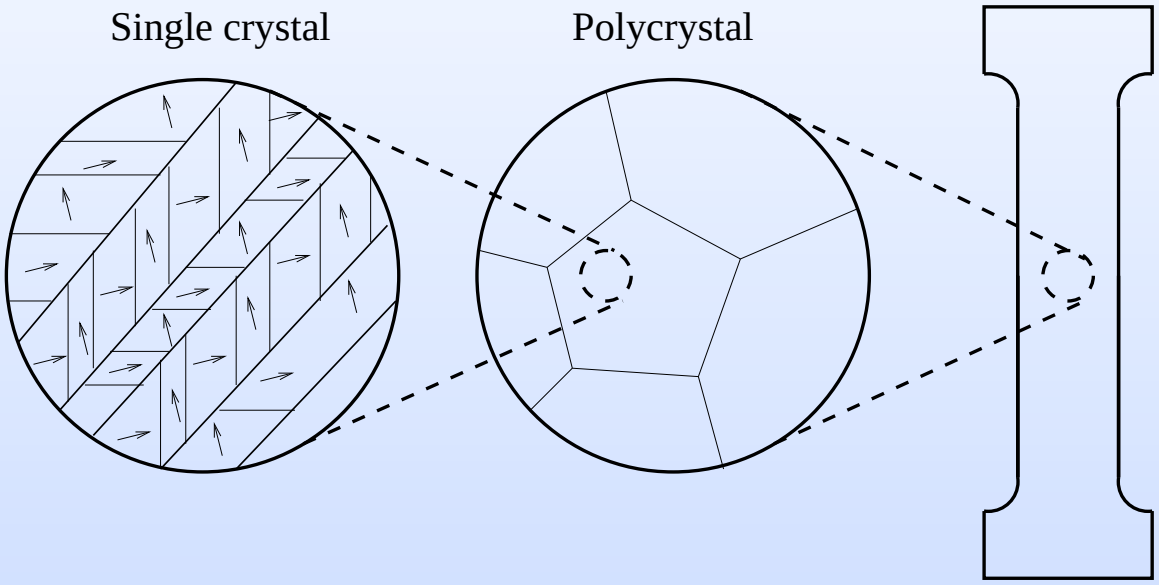
Minimizers and microstructures

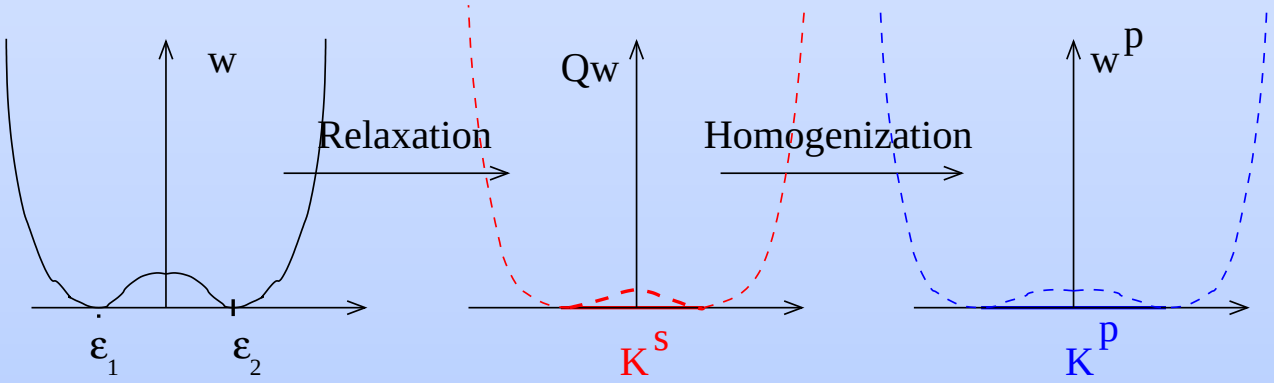




Strain compatibility from one grain to another : strong geometrical constraint.

Energy landscape





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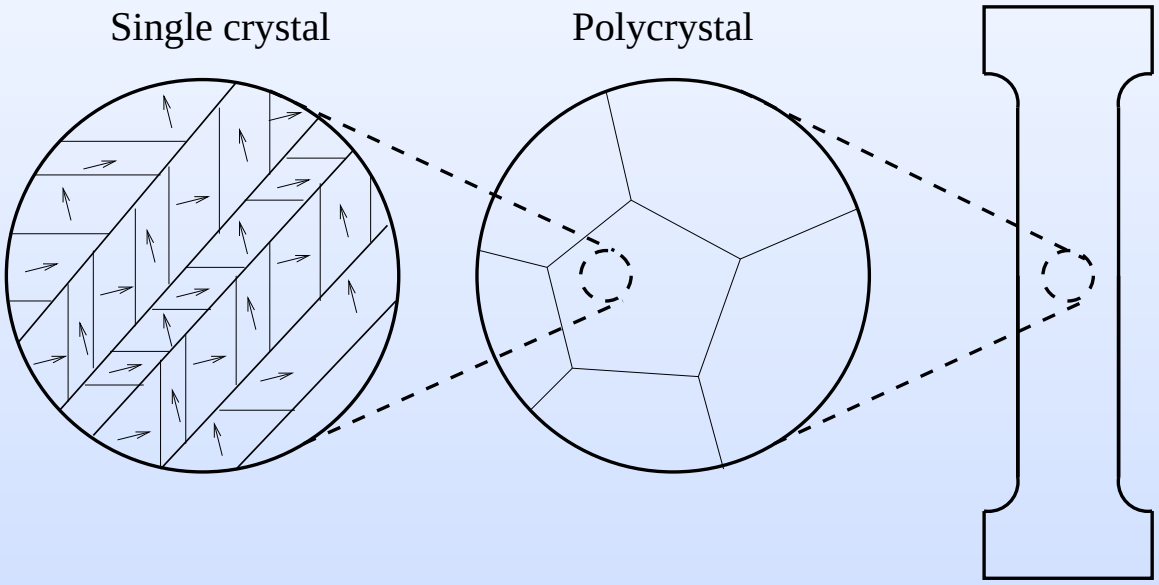
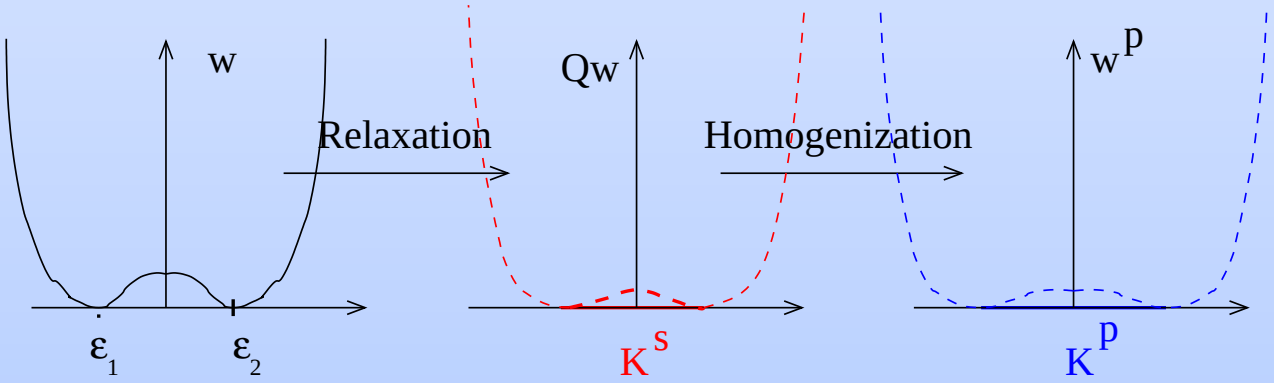


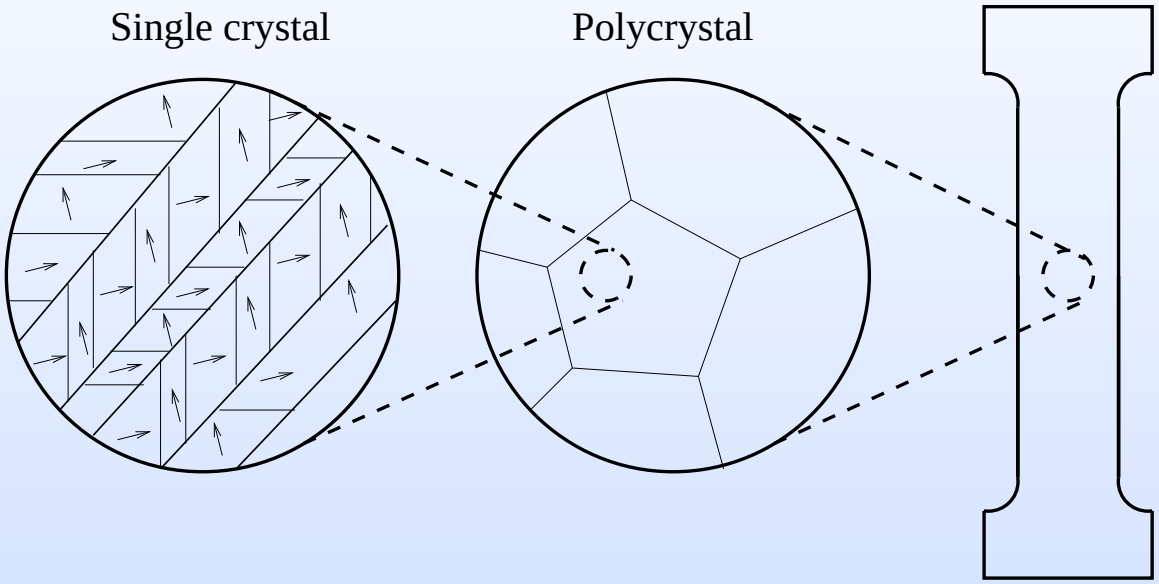


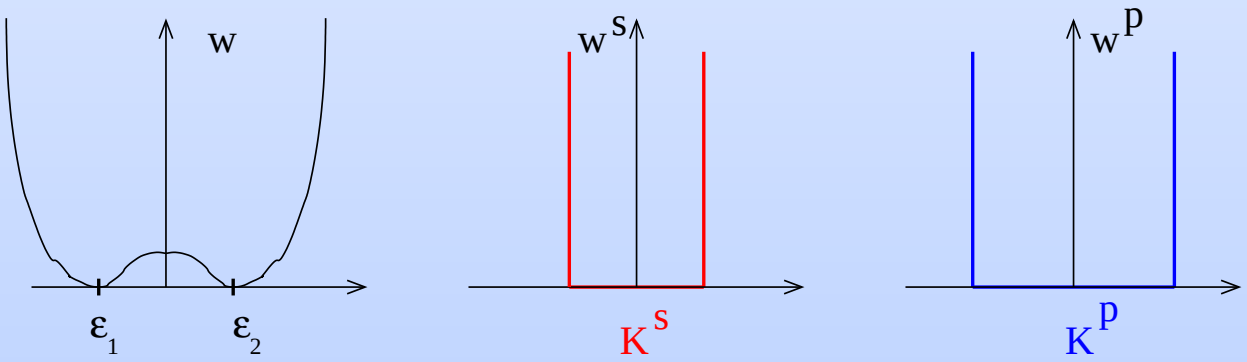
Domains of recoverable strains (strains with $\simeq$ zero energy) :

- ε_1 and ε_2 for the variants,
- K^s for the single crystal,
- K^p for the polycrystal.

Predict K^p from K^s ?

Simplified modelling





Approximations :

- Inside K^s :

$$w^s(\varepsilon) \simeq 0.$$

- Outside K^s :

$$w^s(\varepsilon) \gg 1.$$

- **Replace $w^s = Qw$ by the indicator function of K^s :**

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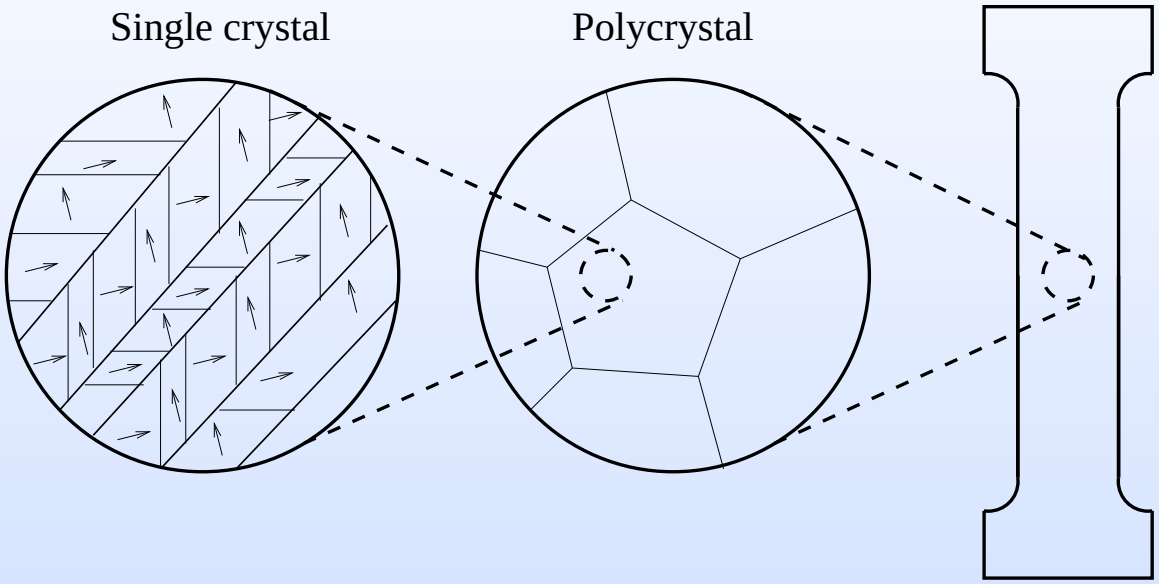
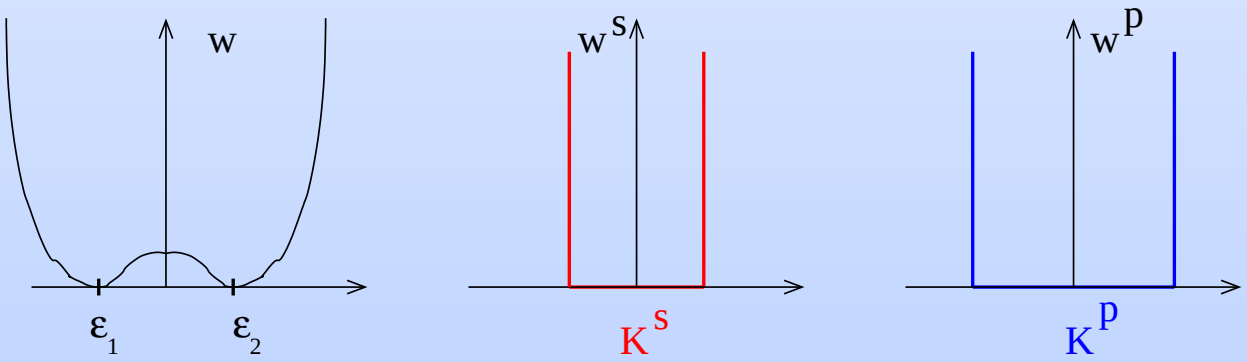
Simplified modelling





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Locking materials (Demengel and PS, 1985) : can deform freely in the interior of K^s but lock on ∂K^s.

Homogenization problem

- **Homogenization problem for a convex energy :**

$$w^p(\overline{\boldsymbol{\varepsilon}}) = \inf_{\boldsymbol{u}\in\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} < w^s(\boldsymbol{R}(\boldsymbol{x}), \boldsymbol{\varepsilon}(\boldsymbol{u})) >, \quad K^p = \{\overline{\boldsymbol{\varepsilon}}, \quad w^p(\overline{\boldsymbol{\varepsilon}}) < +\infty. \}.$$

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- **Dual formulation :**

$$(w^*)^p(\overline{\boldsymbol{\sigma}}) = \inf_{\mathrm{div}(\boldsymbol{\sigma})=0, \langle\boldsymbol{\sigma}\rangle=\overline{\boldsymbol{\sigma}}} < (w^*)^s(\boldsymbol{R}(\boldsymbol{x}), \boldsymbol{\sigma}) > .$$

- $(w^*)^s$ is positively homogeneous of degree 1 in $\boldsymbol{\sigma}$. **Stress with finite energy can be measures concentrated on lines (2d) or surfaces (3d) : locking lines carrying the stress**.

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- The problem is analogous (even identical in 2d, anti-plane strains) to problems for **non-linear, plastic, composites.**

Bounds and estimates for nonlinear polycrystals

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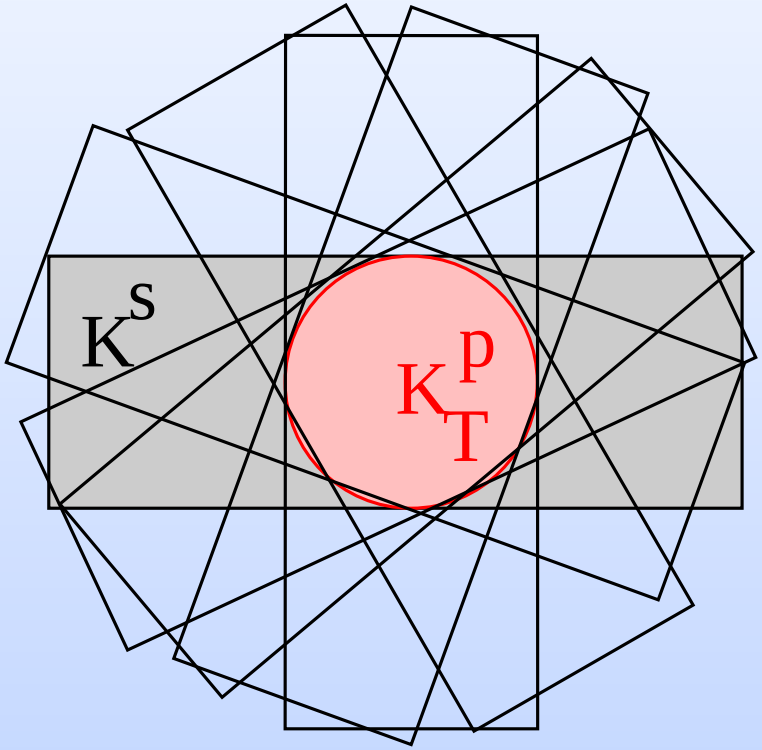

- **Taylor bound :** $\varepsilon = \overline{\varepsilon}$.

$$K^p = \bigcap_{\boldsymbol{x} \in V} K^s(\boldsymbol{R}(\boldsymbol{x})).$$

Locking as soon as the locking condition is attained in one grain. **Very small domain for anisotropic single crystals and untextured polycrystals !**

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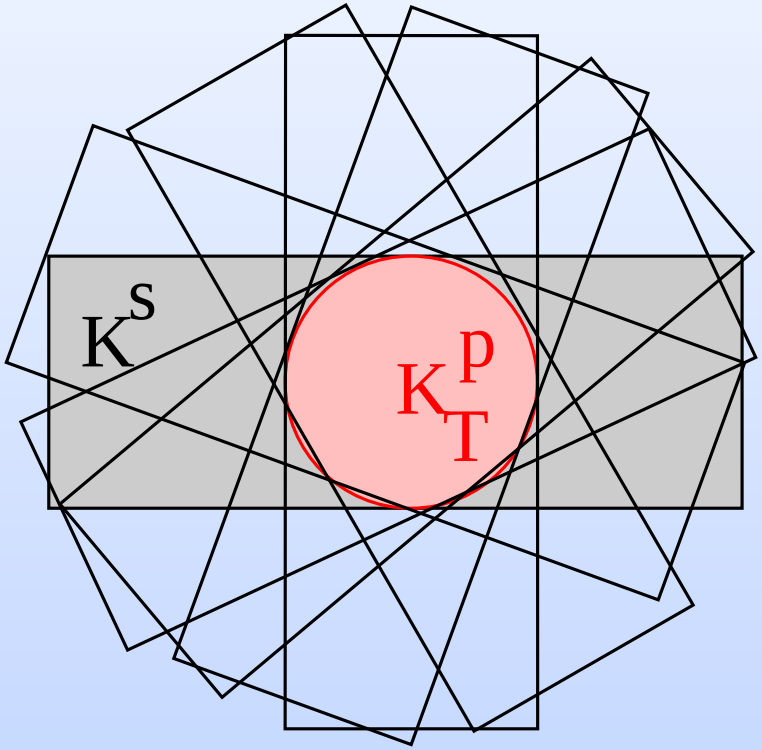

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- **Improved bounds** (Willis 91, Ponte Castañeda 91, PS 92, Olson, 94, Willis, Nesi, Smyshlaev 2000...). Based on the introduction of a **linear comparison composite.**

- **The bounds are far apart** (Taylor is pessimistic, other bounds are optimistic).
- **Objective :** assess the accuracy of various bounds and estimates.

Model Problem (Bhattacharya & Kohn 97)

- **Scalar problem** (antiplane shear) :

$$u(x_1, x_2), \quad \varepsilon_1 = \frac{\partial u}{\partial x_1}, \quad \varepsilon_2 = \frac{\partial u}{\partial x_2}, \quad \frac{\partial \sigma_1}{\partial x_1} + \frac{\partial \sigma_2}{\partial x_2} = 0.$$

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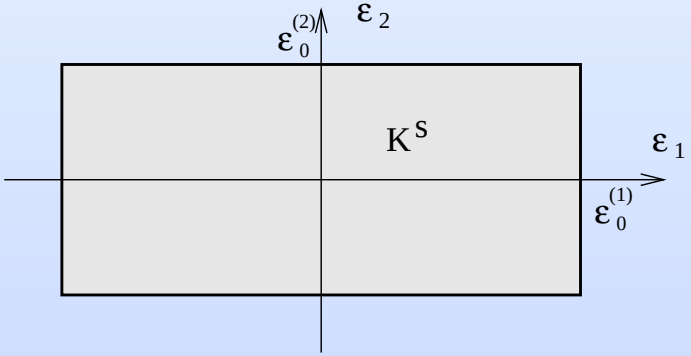
- **Domain of recoverable strains** for the single crystal : $K^s = \{\varepsilon,\ w^s(\varepsilon) = 0\}$.



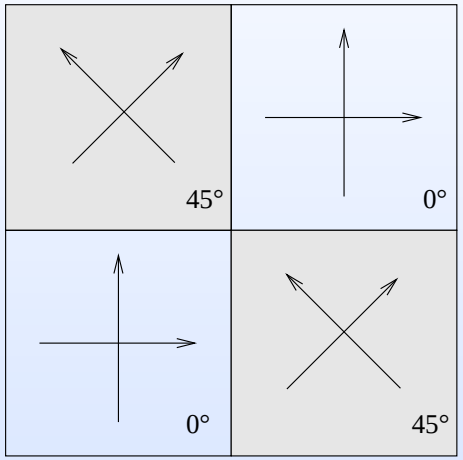
  - 4 “variants”(corners of K^s).
  - If $\varepsilon_0^{(2)} = 0$, only 2 variants.
  - $\varepsilon_0^{(1)}/\varepsilon_0^{(2)} = M$: anisotropy ratio.

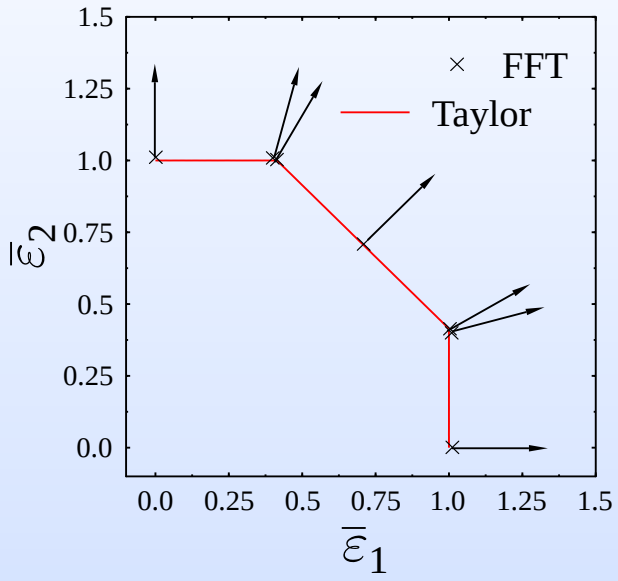
$$|\varepsilon_1| \le \varepsilon_0^{(1)}, \quad |\varepsilon_2| \le \varepsilon_0^{(2)}.$$

- **Dual energy :**

$$(w^*)^s = M|\sigma_1| + |\sigma_2|.$$

Checkerboard bi-crystal. $\varepsilon_0^{(1)} = \varepsilon_0^{(2)} = 1.$





Taylor is exact !

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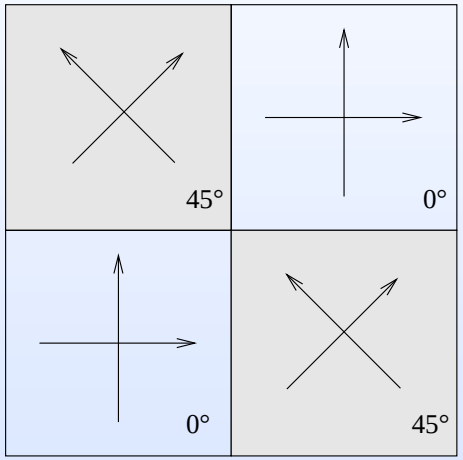
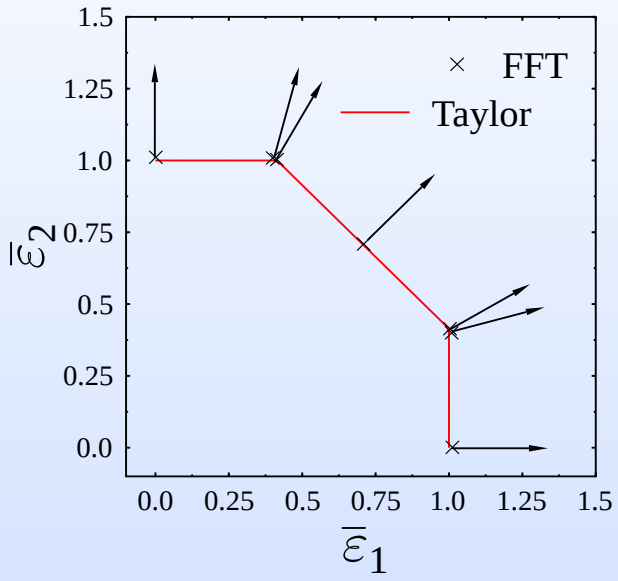
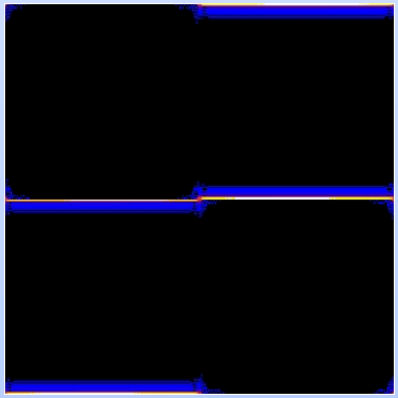


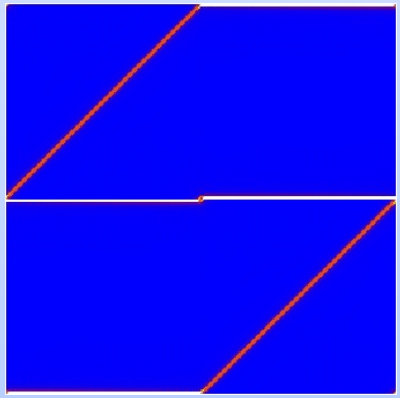


Taylor is exact !

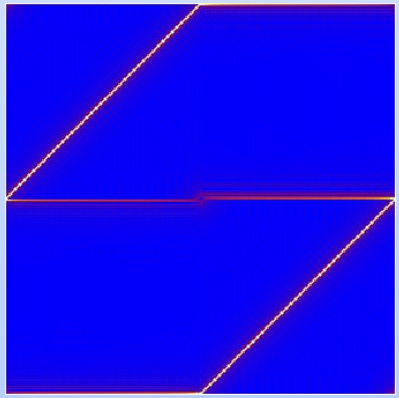
Snapshot of the stress intensity (traction in the direction inclined at angle α :



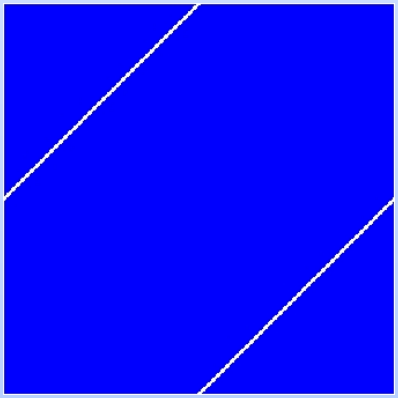
$\alpha = 0^0$



$\alpha = 15^0$

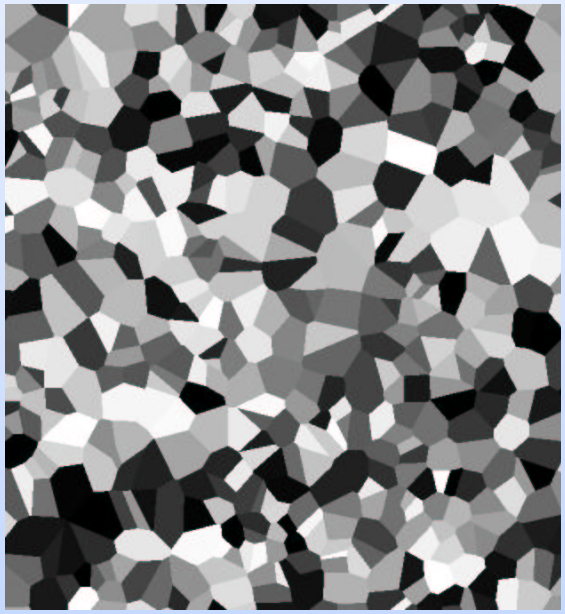


$\alpha = 30^0$

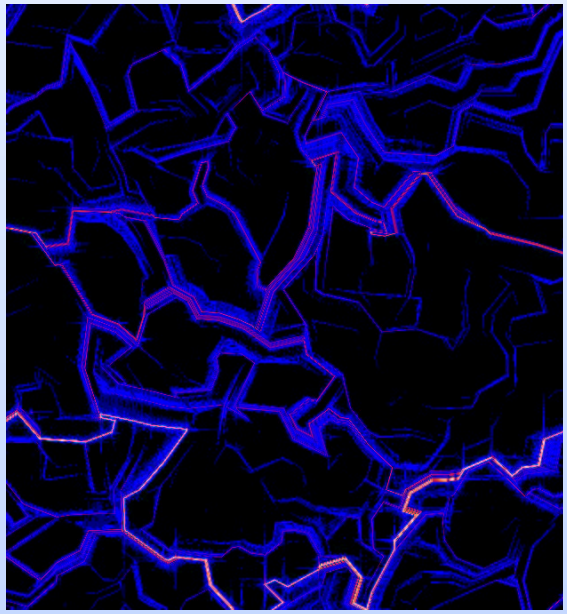


$\alpha = 45^0$

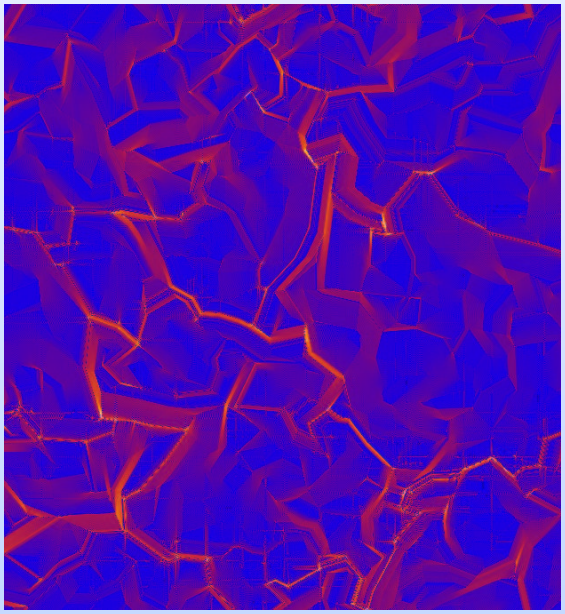
“Locking lines” $M = 50$



Microstructure



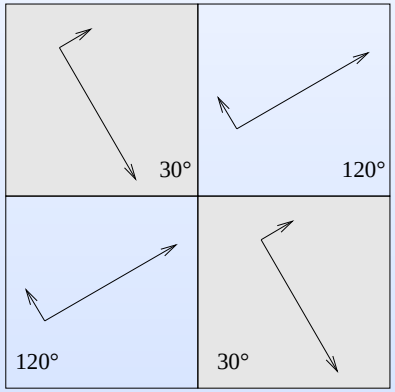
Stress



Strain

Another example of “stress chanelling”

Checkerboard.



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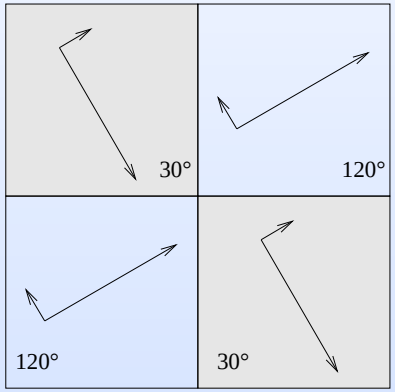

$$(w^s)^* = M|\sigma_1| + |\sigma_2|, \quad M = 10.$$

The stress is chanelled in direction 2 where the transformation strain is small.

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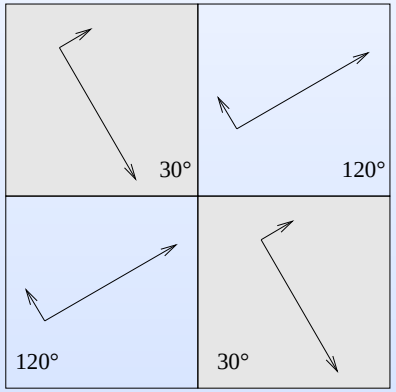

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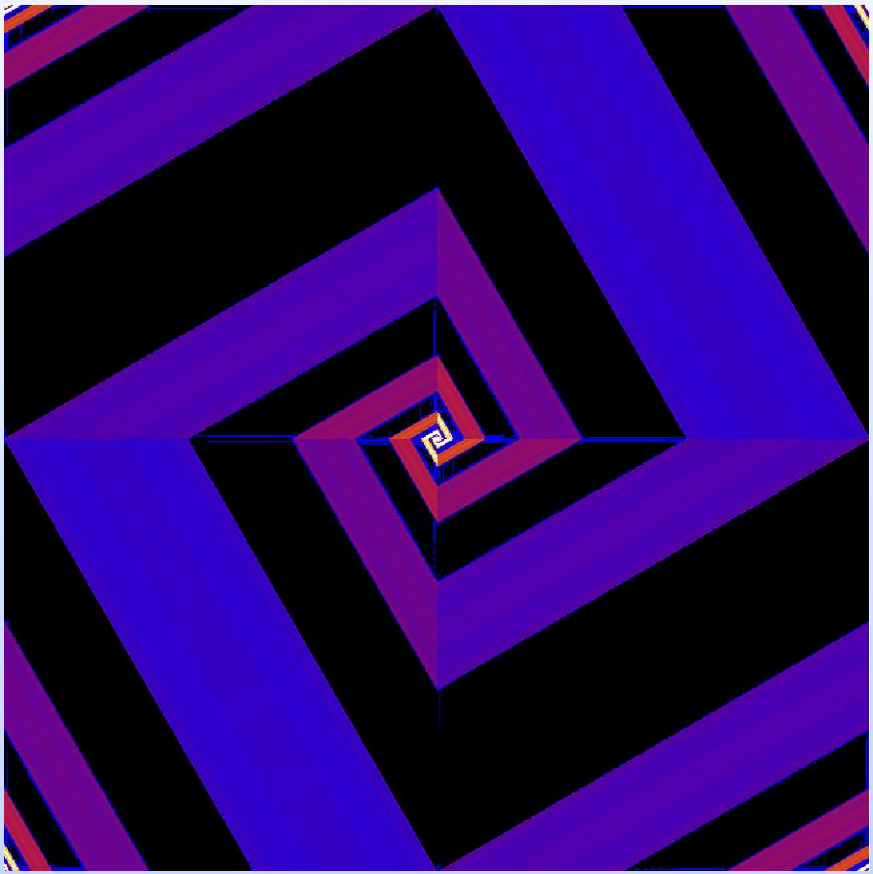
Convexity of the energy does not rule out very fine local fields!

(Not strictly convex).



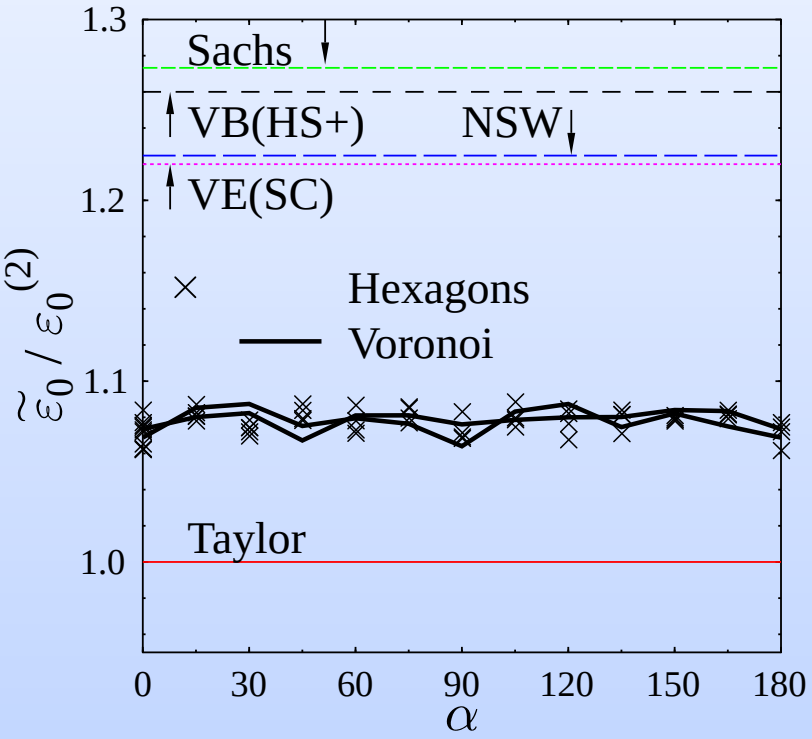
Stress intensity

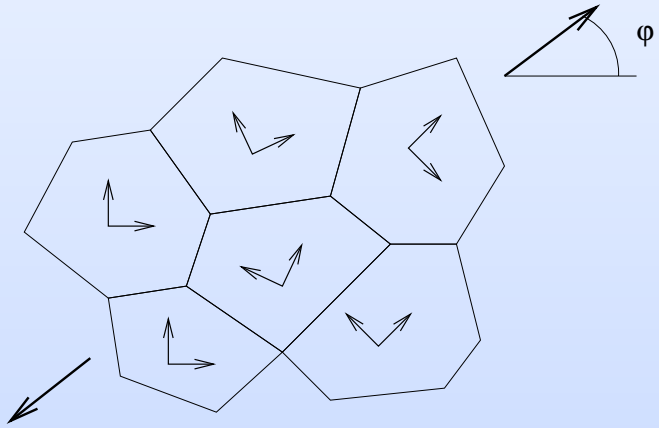
(Spatial resolution 2048 x 2048).

Untextured polycrystals

Untextured : $K^p \simeq$ **isotropic**, radius $\widetilde{\varepsilon}_0$.

Single crystals with "weak" anisotropy $M = \varepsilon_0^{(1)}/\varepsilon_0^{(2)} = 1.$



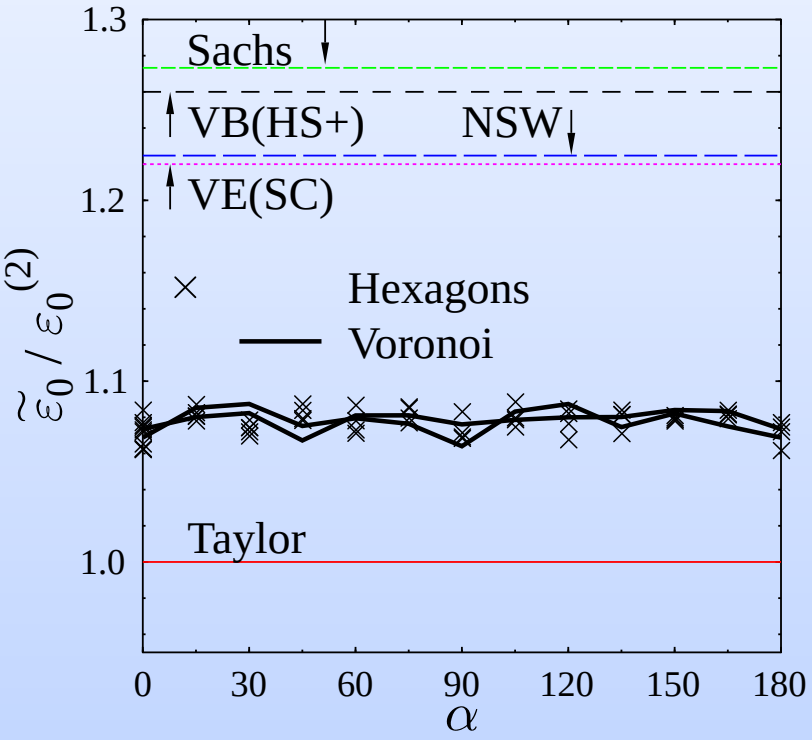


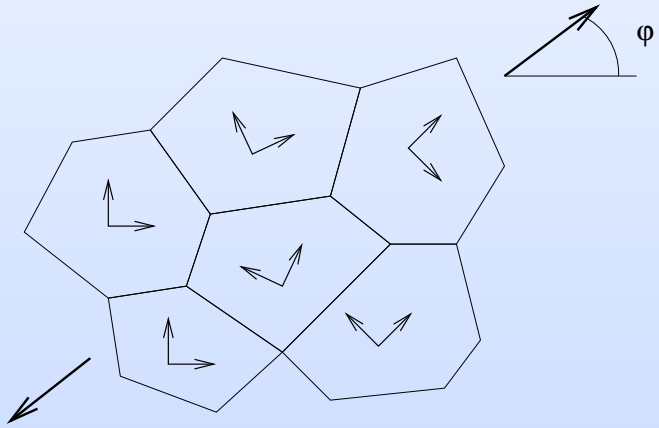
- **Taylor bound :** $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.$
- **FFT :** $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.07.$

Untextured polycrystals

Untextured : $K^p \simeq$ **isotropic**, radius $\widetilde{\varepsilon}_0$.

Single crystals with "weak" anisotropy $M = \varepsilon_0^{(1)}/\varepsilon_0^{(2)} = 1.$



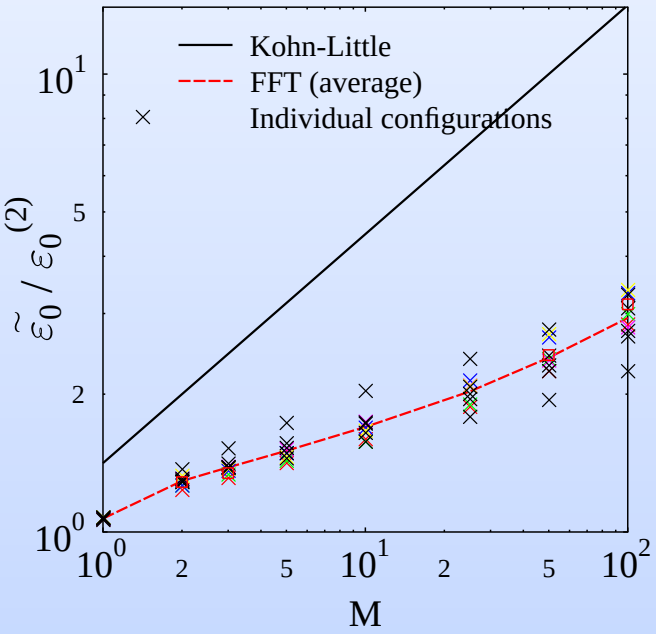


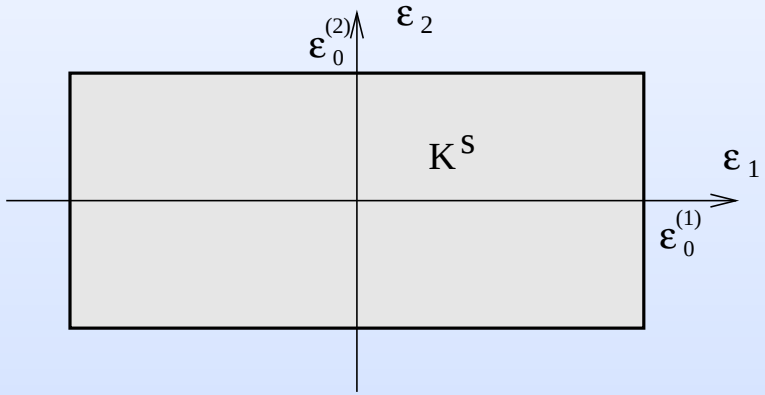
Theoretical predictions :

- Sachs bound : $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 4/\pi \simeq 1.273.$
- Translation bound : $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = \sqrt{3/2} \simeq 1.22.$
- Variational bound : $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.26$
- NIn Self-consistent estimate : $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.22$

- **Taylor bound :** $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.$
- **FFT :** $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.07.$

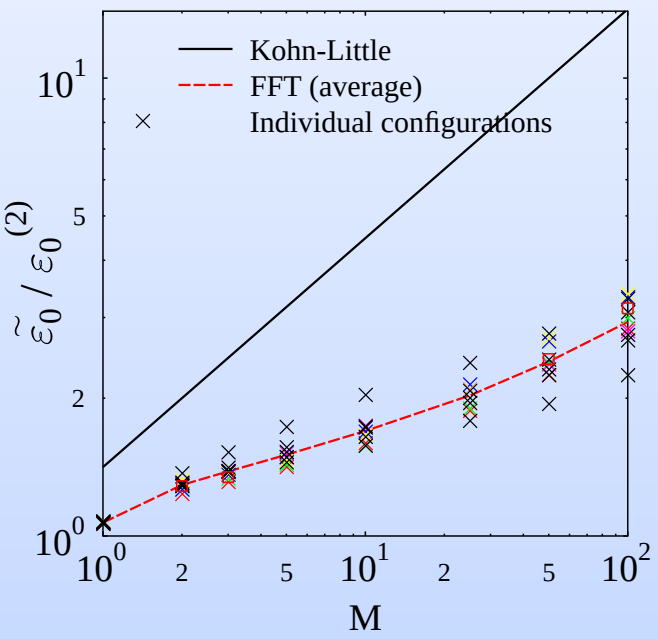
Anisotropic single crystal. $M = \varepsilon_0^{(1)}/\varepsilon_0^{(2)} \neq 1$. Isotropic texture.



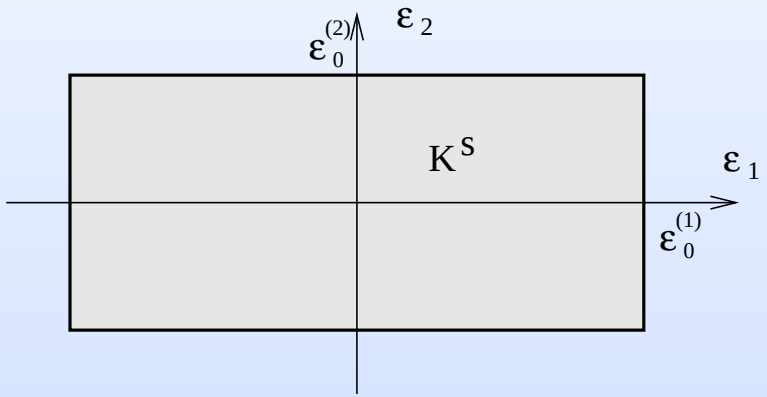


Taylor bound : $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1.$

Anisotropic single crystal. $M = \varepsilon_0^{(1)}/\varepsilon_0^{(2)} \neq 1$. Isotropic texture.



Taylor bound : $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = 1$.



Theoretical predictions :

- Kohn-Little bound $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} = \sqrt{2M}$.
- Nonlinear self-consistent estimate $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} \# \sqrt{M}$.
- Numerical simulations ($1 \leq M \leq 100$) $\widetilde{\varepsilon}_0/\varepsilon_0^{(2)} \# M^{1/4}$.

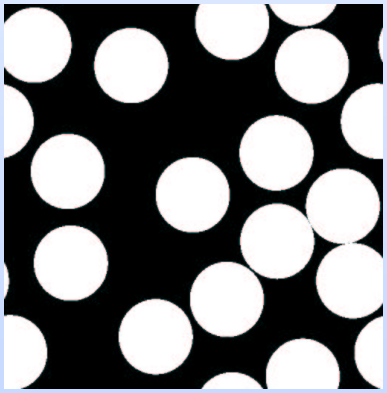
Comments

- Recoverable strains in untextured polycrystals are **significantly smaller** than in single crystals. **Close to the Taylor bound**.
- **Taylor estimate is good for weakly anisotropic materials**, but pessimistic for strongly anisotropic materials.
- **Available general bounds do not seem to predict the right scaling**.
- **Still room for improvement of theoretical estimates**.

5. Estimates for nonlinear composites

Nonlinear local problem

N phases, $r = 1, ..., N$, characteristic functions $\chi^{(r)}$, volume fraction $c^{(r)}$, characterized by their strain-energy function $w^{(r)}$.



Local problem :

Constitutive relations : $\boldsymbol{\sigma}(\boldsymbol{x}) = \frac{\partial w^{(r)}}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}(\boldsymbol{x}))$ dans la phase r,

Equilibrium : $\mathrm{div}(\boldsymbol{\sigma}) = 0$,

Loading : $\langle \boldsymbol{\varepsilon} \rangle = \overline{\boldsymbol{\varepsilon}}$ + Boundary conditions.

Averaging : $\overline{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle$. **Homogenized relations :** $\overline{\boldsymbol{\sigma}}$ as a function of $\overline{\boldsymbol{\varepsilon}}$.

Effective potential

when the $w^{(r)}$'s are (strictly) convex, there exists an effective energy.

$$\widetilde{w}(\overline{\varepsilon}) = \inf_{\boldsymbol{v}\in\mathcal{K}(\overline{\varepsilon})} < w(\boldsymbol{x},\varepsilon(\boldsymbol{v})) >, \qquad \mathcal{K}(\overline{\varepsilon}) = \{\boldsymbol{v} = \overline{\varepsilon}.\boldsymbol{x} + \boldsymbol{v}^*,\ \boldsymbol{v}^* \ \#\ \text{on}\ \partial V\},$$

$$\widetilde{w}^*(\overline{\boldsymbol{\sigma}}) = \inf_{\boldsymbol{\tau}\in\mathcal{S}(\overline{\boldsymbol{\sigma}})} < w^*(\boldsymbol{x},\boldsymbol{\tau} >, \qquad \mathcal{S}(\overline{\boldsymbol{\sigma}}) = \{\boldsymbol{\tau},\ \text{div}(\boldsymbol{\tau}) = 0,\ \langle\boldsymbol{\tau}\rangle = \overline{\boldsymbol{\sigma}},\ \boldsymbol{\tau}.\boldsymbol{n}\ -\#\ \}.$$

Then

$$\overline{\boldsymbol{\sigma}} = \frac{\partial\widetilde{w}}{\partial\overline{\boldsymbol{\varepsilon}}}(\overline{\varepsilon}), \quad \overline{\varepsilon} = \frac{\partial\widetilde{w}^*}{\partial\overline{\boldsymbol{\sigma}}}(\overline{\boldsymbol{\sigma}}).$$

Proof : $\widetilde{w}(\overline{\varepsilon}) = \langle w(\varepsilon(\boldsymbol{u}))\rangle, \quad \dfrac{\partial\widetilde{w}}{\partial\overline{\varepsilon}}(\overline{\varepsilon}) = \left\langle \dfrac{\partial w}{\partial\varepsilon}(\varepsilon(\boldsymbol{u})) : \varepsilon\left(\dfrac{\partial\boldsymbol{u}}{\partial\overline{\varepsilon}}\right)\right\rangle = \left\langle \boldsymbol{\sigma} : \varepsilon\left(\dfrac{\partial\boldsymbol{u}}{\partial\overline{\varepsilon}}\right)\right\rangle.$

$$\langle\varepsilon\rangle = \overline{\varepsilon} \quad \Rightarrow \quad \left\langle \varepsilon\left(\frac{\partial\boldsymbol{u}}{\partial\overline{\varepsilon}}\right)\right\rangle = \boldsymbol{I} \quad \overset{\text{Hill}}{\Rightarrow} \quad \frac{\partial\widetilde{w}}{\partial\overline{\varepsilon}}(\overline{\varepsilon}) = \langle\boldsymbol{\sigma}\rangle : \boldsymbol{I} = \overline{\boldsymbol{\sigma}}.$$

Elementary bounds

Choose $\boldsymbol{v} = \overline{\boldsymbol{\varepsilon}}.\boldsymbol{x}$ and $\boldsymbol{\tau} = \overline{\boldsymbol{\sigma}}$

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}) \leq < w > (\overline{\boldsymbol{\varepsilon}}) \quad \text{(Voigt)}, \quad \widetilde{w}^*(\overline{\boldsymbol{\sigma}}) \leq < w^* > (\overline{\boldsymbol{\sigma}}) \quad \text{(Reuss)}.$$

Power-law materials with the same exponent n (or m), the same ε_0 but different flow stress $\sigma_0^{(r)}$:

$$w^{(r)}(\boldsymbol{\varepsilon}) = \frac{\sigma_0^{(r)}\varepsilon_0}{m+1}\left(\frac{\varepsilon_{\text{eq}}}{\varepsilon_0}\right)^{m+1}, \quad \widetilde{w}(\overline{\boldsymbol{\varepsilon}}) = \frac{\widetilde{\sigma}_0\varepsilon_0}{m+1}\left(\frac{\overline{\varepsilon}_{\text{eq}}}{\varepsilon_0}\right)^{m+1},$$

$$< \sigma_0^{-1/n} >^{-n} \leq \widetilde{\sigma}_0 \leq < \sigma_0 >$$

Rigid-plastic materials ($m = 0, n = +\infty$)

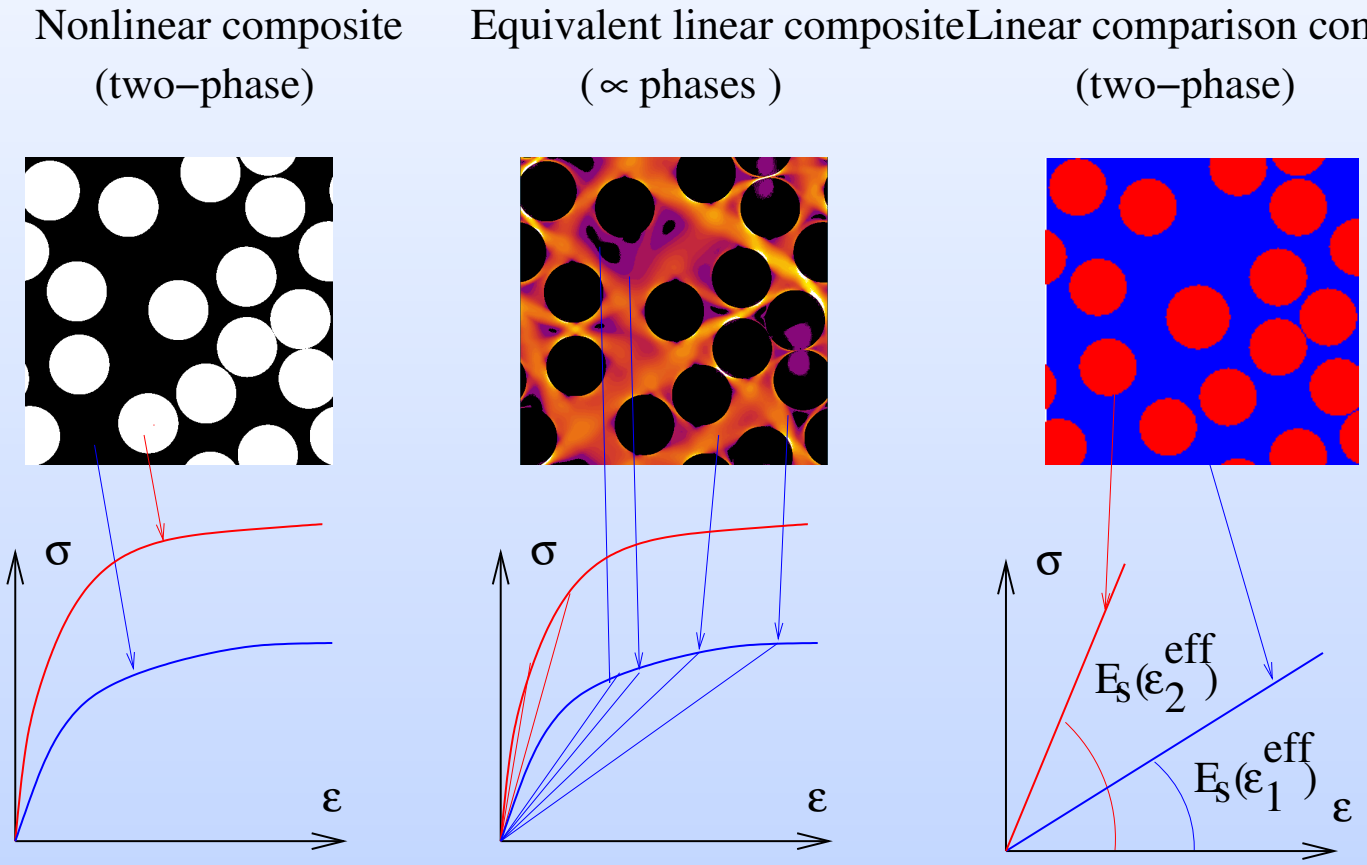
$$\inf_{(r)} \sigma_0^{(r)} \leq \widetilde{\sigma}_0 \leq < \sigma_0 > .$$

Weakest link property.

Objective : improve on these bounds.

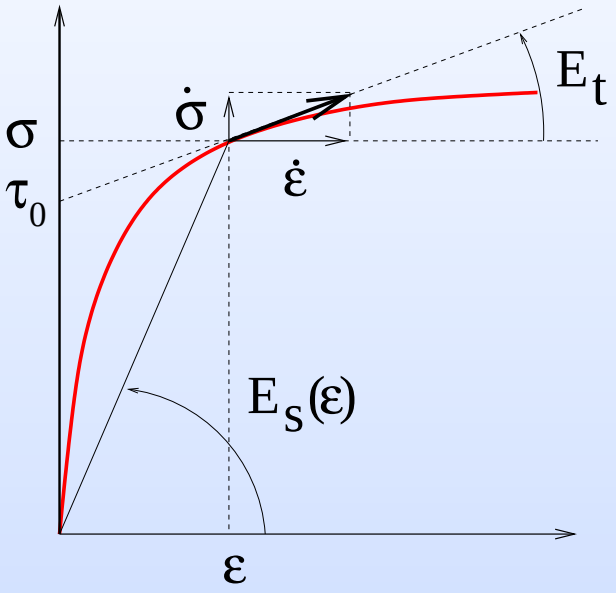
Heuristic methods : Linear Comparison Composite

A nonlinear composite behaves as a linear composite with infinitely many different phases.



Approximation= replace the N-phase nonlinear composite by a N-phase linear composite :

Choose a linearization rule



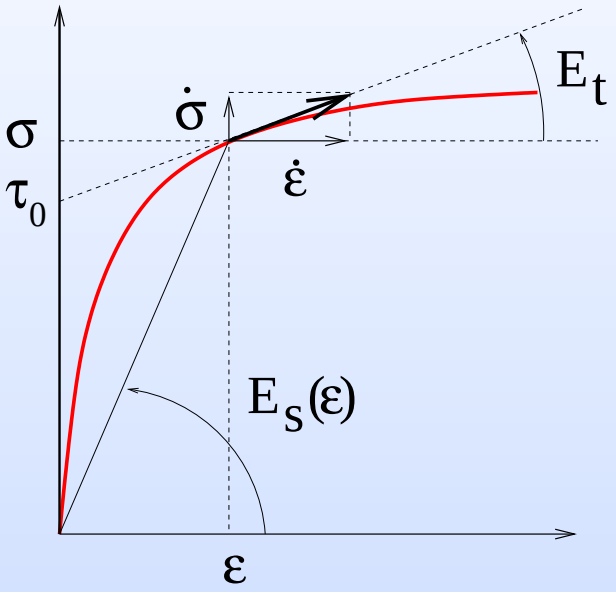
- **Secant formulation :**

$$\boldsymbol{\sigma} = \boldsymbol{L}_{\text{sct}}(\boldsymbol{\varepsilon}) : \boldsymbol{\varepsilon}.$$

- **Tangent (or incremental) formulation :**

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{L}_{\text{tgt}}(\boldsymbol{\varepsilon}) : \dot{\boldsymbol{\varepsilon}}.$$

Choose a linearization rule



- **Secant formulation :**

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- **Tangent (or incremental) formulation :**

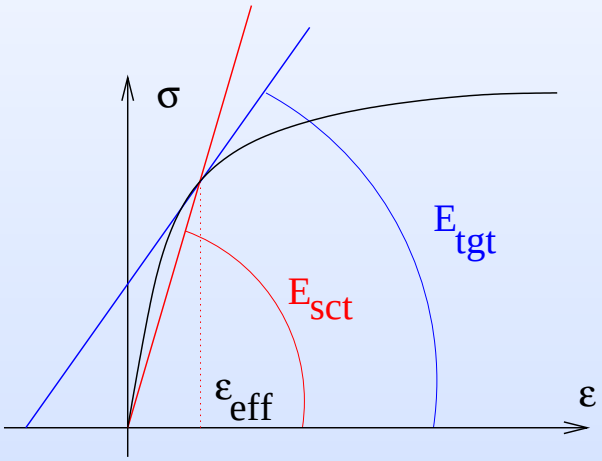
$$\dot{\boldsymbol{\sigma}} = \boldsymbol{L}_{\text{tgt}}(\boldsymbol{\varepsilon}) : \dot{\boldsymbol{\varepsilon}}.$$

Define an effective strain (stress)

The stiffness of the LCC is the (secant or tangent) stiffness of the actual nonlinear composite evaluated at some **effective strain** $\boldsymbol{\varepsilon}_{\text{eff}}^{(r)}$ for each individual phase.

Is the strain uniform in the phase ? If not, define an “optimal” effective strain.

Effective strain : the most classical and simplest choice

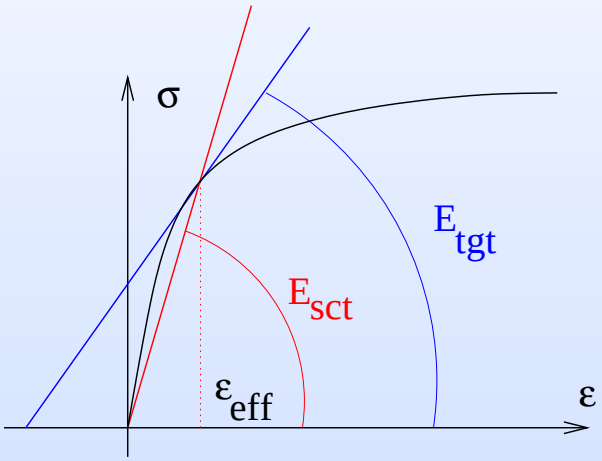


Mean field theories : effective strain = average strain.

$$\varepsilon_{\text{eff}}^{(r)} = \overline{\varepsilon}^{(r)} = \langle \varepsilon \rangle_r .$$

Good if the strain field is almost uniform with each individual phase.

Effective strain : the most classical and simplest choice



Mean field theories : effective strain = average strain.

$$\varepsilon_{\text{eff}}^{(r)} = \overline{\varepsilon}^{(r)} = \langle \varepsilon \rangle_r .$$

Good if the strain field is almost uniform with each individual phase.

Aim of the rest of this talk :

- Show that **the strain field (or the plastic strain field) is far from being uniform** in each individual phase or grain (intraphase heterogeneity).
- Use numerical simulation to get an insight into the **intraphase fluctuations.**
- Propose **an *ad hoc* model** accounting for the intrinsic nonuniformity of the plastic strain field.

Rigorous approach : variational procedure (Ponte Castañeda 92)

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}) = \inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \langle w(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v})) \rangle .$$

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Linear Comparison Composite with quadratic energy w_0 :

$$w_0(\boldsymbol{x}, \boldsymbol{\varepsilon}) = \frac{1}{2} \boldsymbol{\varepsilon} : \boldsymbol{L}_0(\boldsymbol{x}) : \boldsymbol{\varepsilon}.$$

Translation :

$$\widetilde{w}(\overline{\boldsymbol{\varepsilon}}) = \inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\boldsymbol{\varepsilon}})} < w(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v})) > = \inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\boldsymbol{\varepsilon}})} (< w_0(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v})) > + < (w - w_0)(\boldsymbol{x}, \boldsymbol{\varepsilon}(\boldsymbol{v}))$$

Rigorous approach : variational procedure (Ponte Castañeda 92)

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$$\leq \left(\inf_{\boldsymbol{v}\in\mathcal{K}(\overline{\boldsymbol{\varepsilon}})} \langle w_0(\boldsymbol{x},\boldsymbol{\varepsilon}(\boldsymbol{v}))\rangle\right) + \left\langle \sup_{\boldsymbol{e}\in\boldsymbol{R}^9_s} (w-w_0)(\boldsymbol{x},e)\right\rangle$$

$$\leq \frac{1}{2}\overline{\boldsymbol{\varepsilon}} : \widetilde{\boldsymbol{L}}_0 : \overline{\boldsymbol{\varepsilon}} + \langle V(\boldsymbol{L}_0)\rangle \quad \forall\, \boldsymbol{L}_0 > 0, \quad V(\boldsymbol{L}_0) = \sup_{\boldsymbol{e}\in\boldsymbol{R}^9_s} (w-w_0)(\boldsymbol{x},e)$$

Rigorous approach : variational procedure (Ponte Castañeda 92)

$$\widetilde{w}(\overline{\varepsilon}) = \inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\varepsilon})} \langle w(\boldsymbol{x}, \varepsilon(\boldsymbol{v})) \rangle .$$

Linear Comparison Composite with quadratic energy w_0 :

$$w_0(\boldsymbol{x}, \varepsilon) = \frac{1}{2} \varepsilon : \boldsymbol{L}_0(\boldsymbol{x}) : \varepsilon .$$

Translation :

$$\widetilde{w}(\overline{\varepsilon}) = \inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\varepsilon})} < w(\boldsymbol{x}, \varepsilon(\boldsymbol{v})) > = \inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\varepsilon})} (< w_0(\boldsymbol{x}, \varepsilon(\boldsymbol{v})) > + < (w - w_0)(\boldsymbol{x}, \varepsilon(\boldsymbol{v}))$$

$$\leq \left(\inf_{\boldsymbol{v} \in \mathcal{K}(\overline{\varepsilon})} \langle w_0(\boldsymbol{x}, \varepsilon(\boldsymbol{v})) \rangle \right) + \left\langle \sup_{\boldsymbol{e} \in \boldsymbol{R}_s^9} (w - w_0)(\boldsymbol{x}, e) \right\rangle$$

$$\leq \frac{1}{2} \overline{\varepsilon} : \widetilde{\boldsymbol{L}}_0 : \overline{\varepsilon} + \langle V(\boldsymbol{L}_0) \rangle \quad \forall \, \boldsymbol{L}_0 > 0, \quad V(\boldsymbol{L}_0) = \sup_{\boldsymbol{e} \in \boldsymbol{R}_s^9} (w - w_0)(\boldsymbol{x}, e)$$

$$\leq \inf_{\boldsymbol{L}_0(\boldsymbol{x})} \left(\frac{1}{2} \overline{\varepsilon} : \widetilde{\boldsymbol{L}}_0 : \overline{\varepsilon} + \langle V(\boldsymbol{L}_0) \rangle \right) \quad \textbf{Optimal choice for } \boldsymbol{L}_0 .$$

6. Field fluctuations

In linear composites, it is sufficient to determine the first moment (average) of the strain over each phase : $\overline{\varepsilon}_r = \boldsymbol{A}_r : \overline{\varepsilon}$.

$$\overline{\boldsymbol{\sigma}} = \sum_{r=1}^{N} c^{(r)} \overline{\boldsymbol{\sigma}}_r = \sum_{r=1}^{N} c^{(r)} \boldsymbol{L}^{(r)} : \overline{\varepsilon}_r \quad \Rightarrow \quad \overline{\boldsymbol{\sigma}} = \left(\sum_{r=1}^{N} c^{(r)} \boldsymbol{L}^{(r)} : \boldsymbol{A}_r \right) : \overline{\varepsilon}$$

This is NO more the case for nonlinear composites :

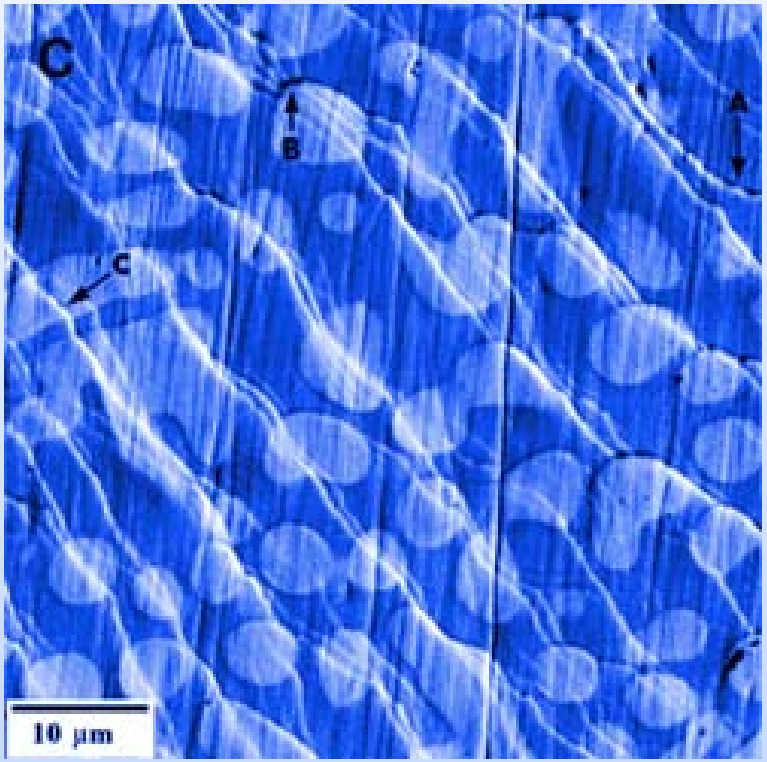
$$\boldsymbol{\sigma} = \mathcal{F}^{(r)}(\varepsilon), \quad \textbf{BUT} \quad \overline{\boldsymbol{\sigma}}^{(r)} \neq \mathcal{F}^{(r)}(\overline{\varepsilon}^{(r)}).$$

The local fields have to be fully resolved !

$$\varepsilon(\boldsymbol{x}) = \underbrace{\overline{\varepsilon}_r}_{\textbf{Mean field}} + \underbrace{(\varepsilon(\boldsymbol{x}) - \overline{\varepsilon}_r)}_{\textbf{Fluctuation}}.$$

Average of fluctuations = 0. **intensity of fluctuations measured by their2nd moment (covariance).**

Experimental evidence of intraphase strain heterogeneity

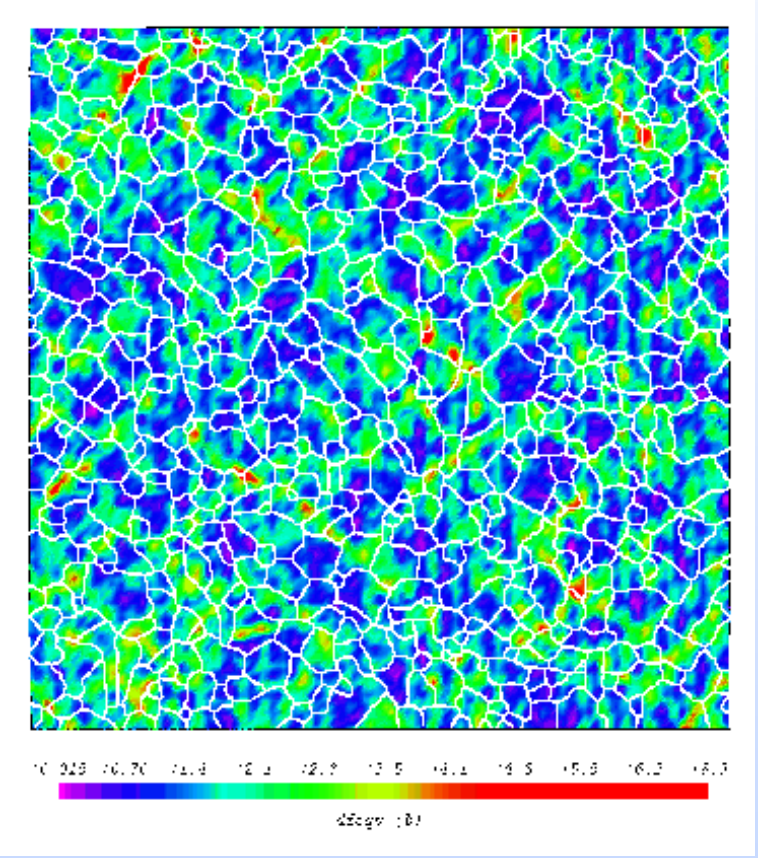


Bulk metallic glass.

- Amorphous matrix. Crystalline inclusions.
- Uniaxial tension in the vertical direction.
- Optical microscopy.
- Strain localization initiated in the crystalline inclusions, running through the matrix.
- Inclination of the most deformed zones (shear bands in white) at 45^0.

©W. Johnson (Caltech, USA)

The strain field is far from being uniform in each phase : **Intraphase heterogeneity : heterogeneity with a single phase.**



Polycrystalline Zirconium.

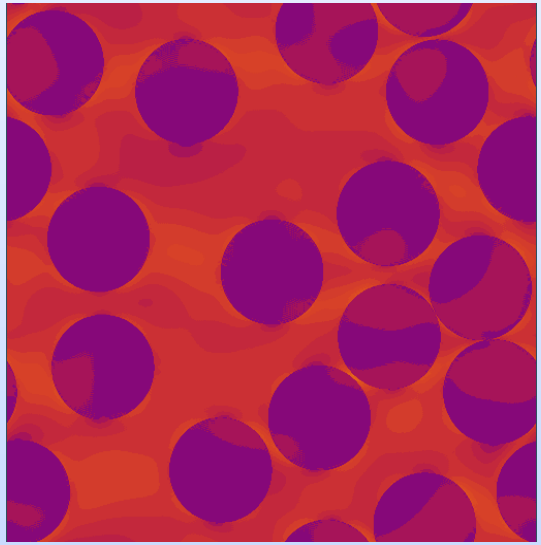
- Grain boundaries (white).
- Uniaxial tension in the vertical direction. Overall deformation 3.5%.
- Observation (SEM) during test. Microextensometry using a microgrid with a 5μm step.
- Snapshot of the equivalent strain.
- Inclination of the most deformed zones at $\pm 45^0$.

©P. Doumalin, M. Bornert (Ecole Polytechnique, France)

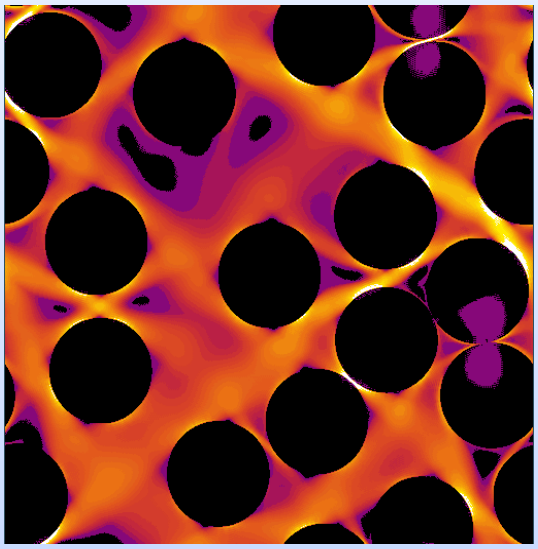
The strain field is far from being uniform in each grain !

Strain heterogeneity seen through numerical simulation

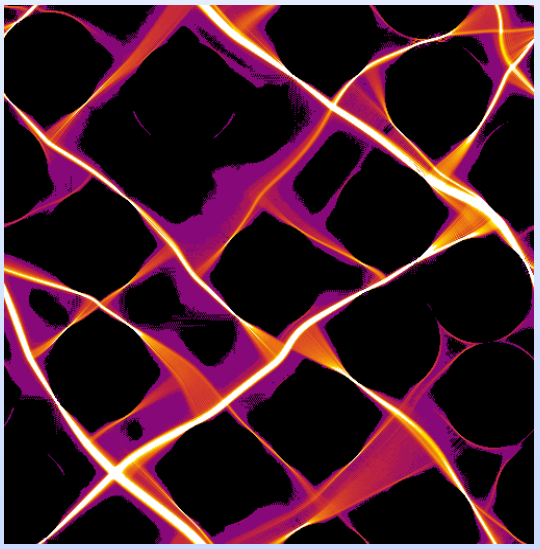
Influence of the matrix nonlinearity on the strain heterogeneity within the matrix (intraphase strain heterogeneity). Elastic fibers, nonlinear matrix. Tension in the horizontal direction. Generalized plane strains.



Matrix : linear elastic



... with linear hardening



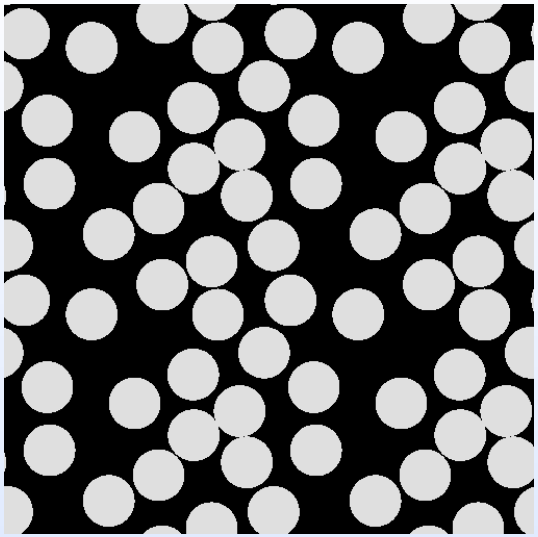
ideally plastic

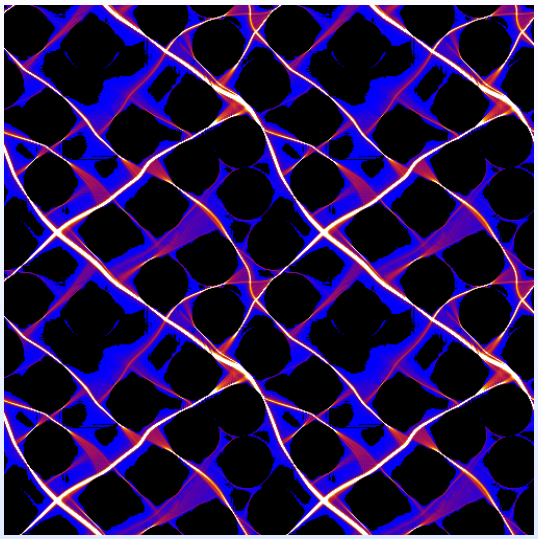
Conclusion : the strain field (in the matrix) is close to uniform when the matrix is linear elastic, not too far from uniform for a matrix with linear hardening, highly localized (heterogeneous) when the matrix is elastic perfectly plastic.

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.

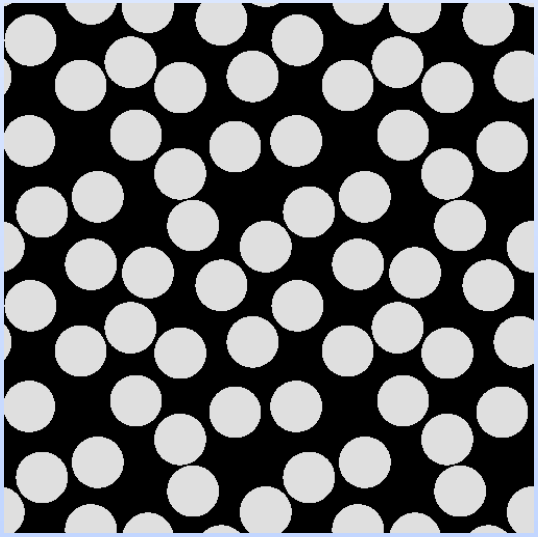


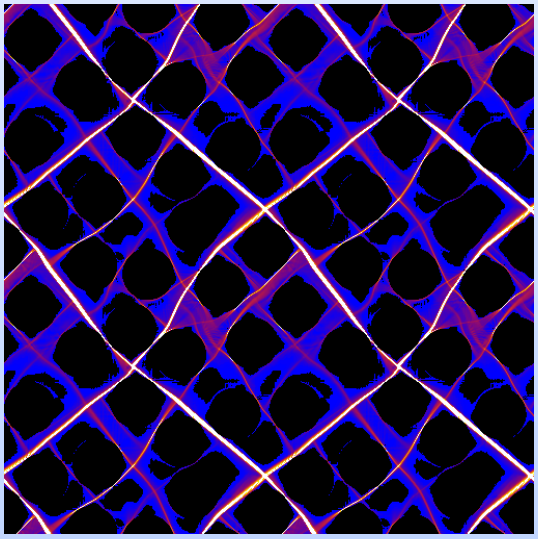


"Weak" configuration. More regular spatial arrangement. Shear bands running at $\pm 45^0$ with respect to the tensile direction.

"Low" flow stress.

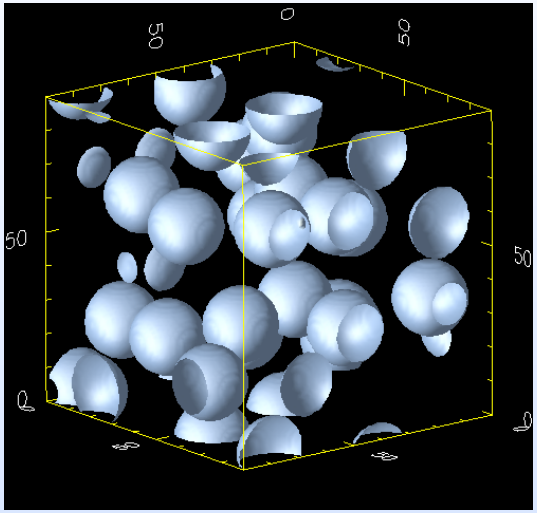
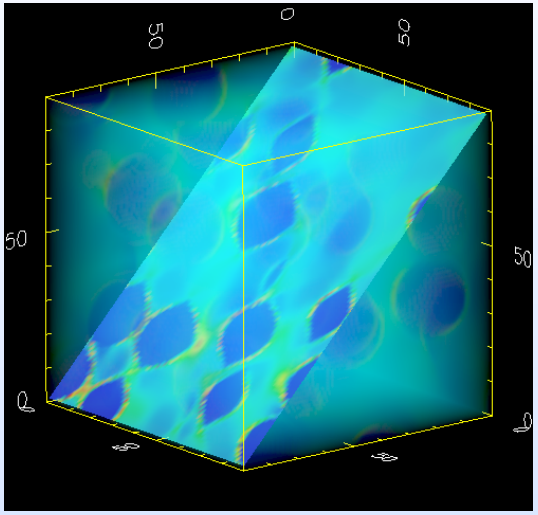
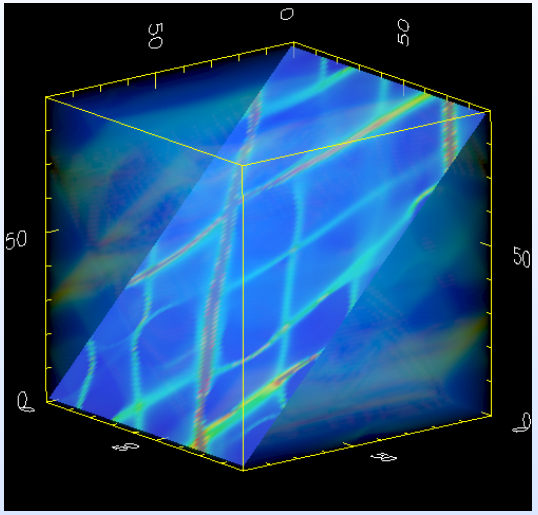
Percolation of shear bands.

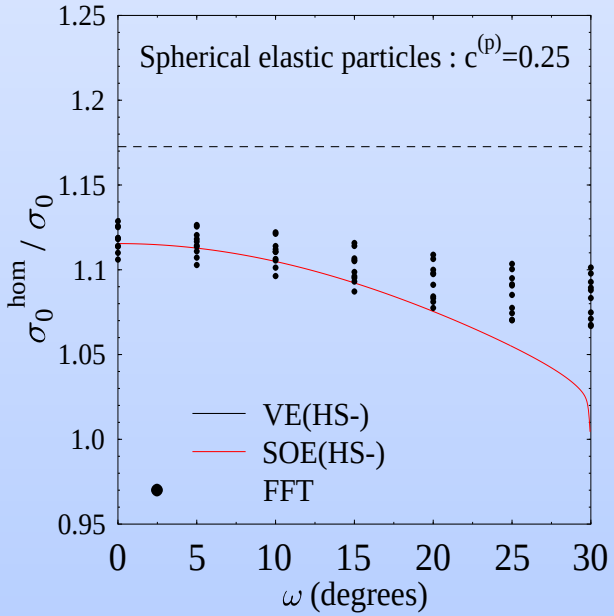




The composite effective properties are not governed by the volume fraction of the fibers but by the tortuosity of the matrix domain.

Similar effects in 3d



Elastic inclusions. Ideally plastic matrix.

Uniaxial tension

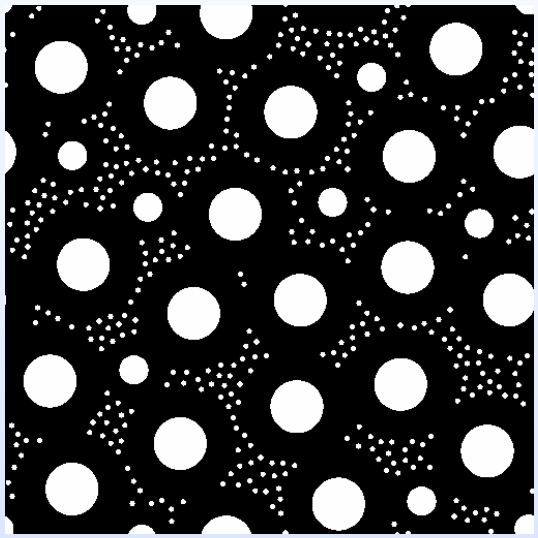
$$\overline{\boldsymbol{\sigma}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \overline{\sigma}_{\text{eq}} \end{pmatrix}$$

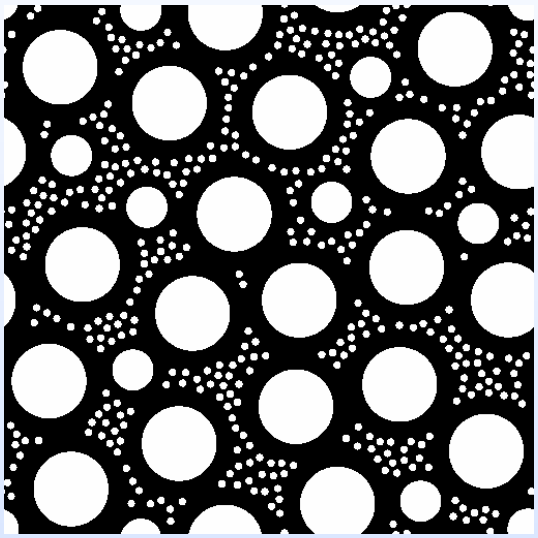
Pure shear

$$\overline{\boldsymbol{\sigma}} = \frac{1}{\sqrt{3}} \begin{pmatrix} \overline{\sigma}_{\text{eq}} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\overline{\sigma}_{\text{eq}} \end{pmatrix}$$

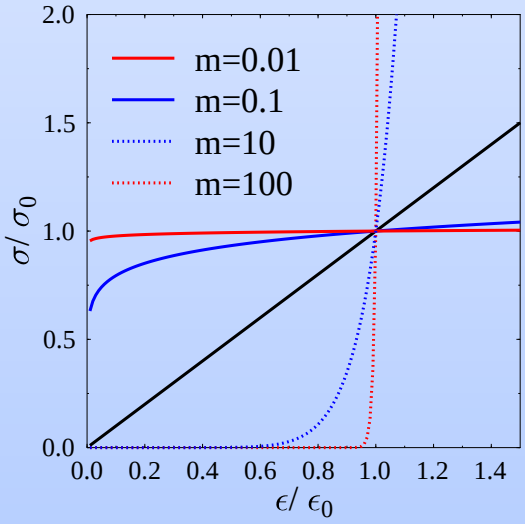
Highly localized strain field $\Rightarrow$ lower flow stress for the composite.

How does the intraphase strain heterogeneity depend on nonlinearity ?





Inclusion-matrix microstructures, power-law and incompressible phases.



$$\mathrm{tr}\,(\boldsymbol{\varepsilon}) = 0, \quad \frac{\boldsymbol{\varepsilon}}{\varepsilon_{\mathrm{eq}}} = \frac{2}{3}\frac{\boldsymbol{s}}{\sigma_{\mathrm{eq}}}, \quad \boldsymbol{s} \ : \ \text{stress deviator},$$

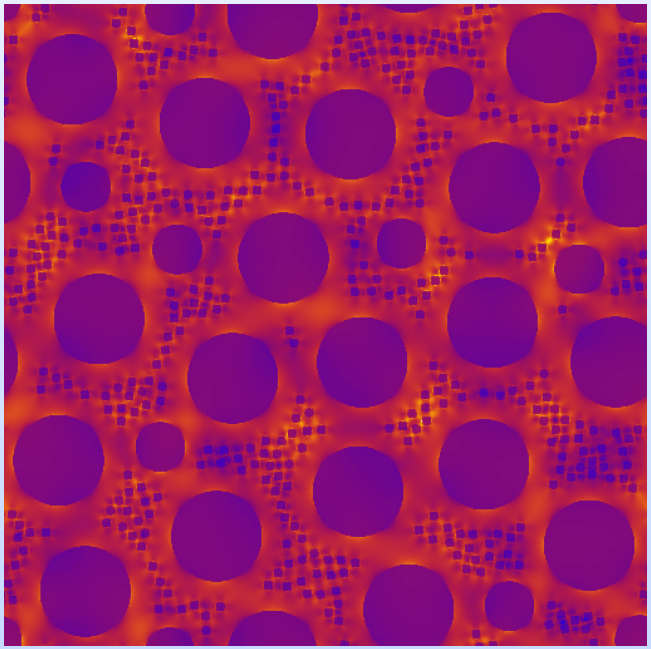
$$\sigma_{\mathrm{eq}} = \sigma_0 \left(\frac{\varepsilon_{\mathrm{eq}}}{\varepsilon_0}\right)^m, \quad \varepsilon_{\mathrm{eq}} = \varepsilon_0 \left(\frac{\sigma_{\mathrm{eq}}}{\sigma_0}\right)^n, \quad n = \frac{1}{m},$$

$m = 1, n = 1$: linear elastic, $m = 0, n = +\infty$: rigid plastic material.

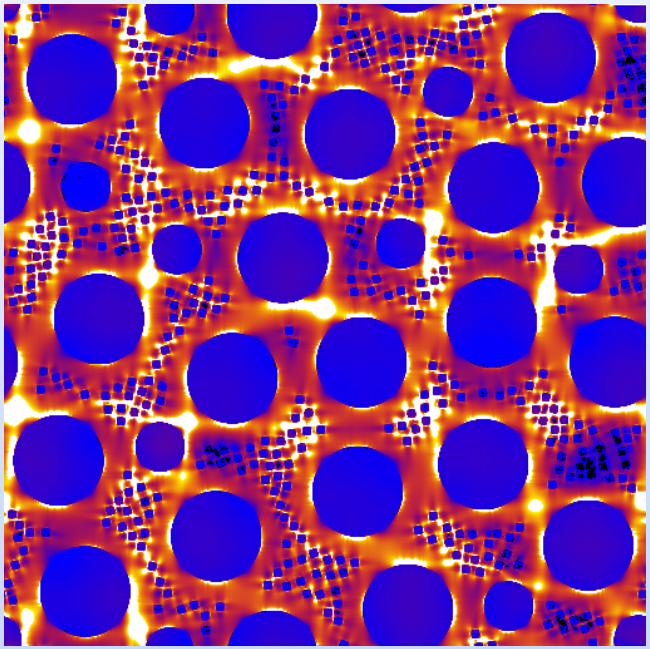
n measures the material nonlinearity.

Strain fields

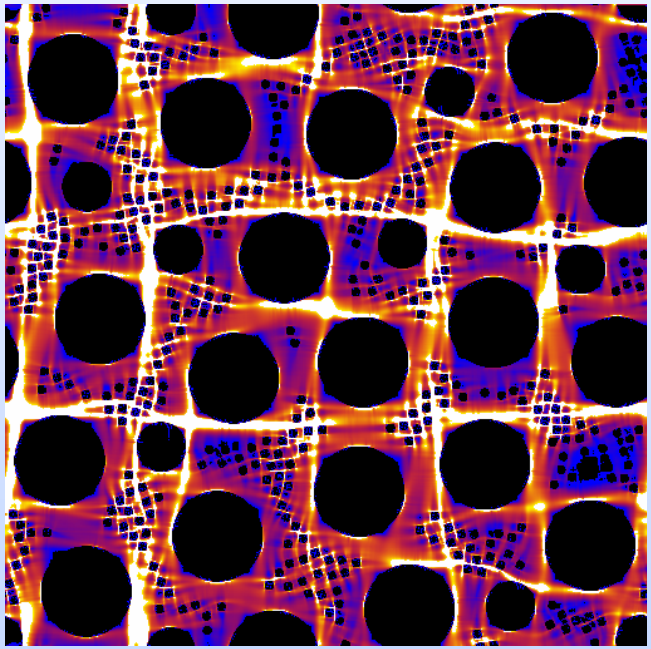
- Same exponent n for both phases but different flow stresses σ_0. $\sigma_0^{(1)}/\sigma_0^{(2)} = 5$.
- Applied loading : pure shear $\overline{\varepsilon}_{12} \neq 0$, other $\overline{\varepsilon}_{ij} = 0$. Snapshot of ε_{12}. Same color scale for all snapshots.



$n = 1$



$n = 3$

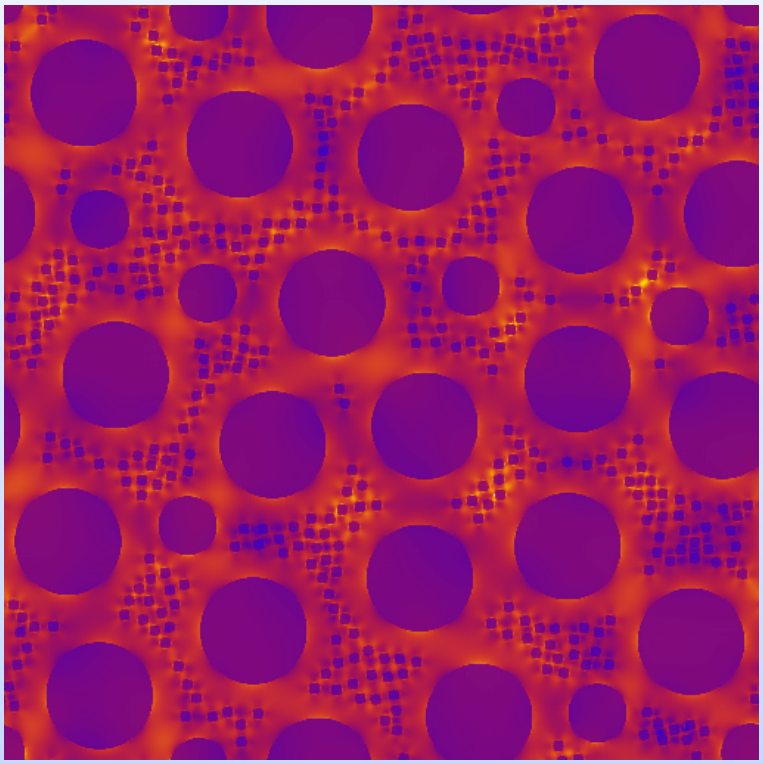


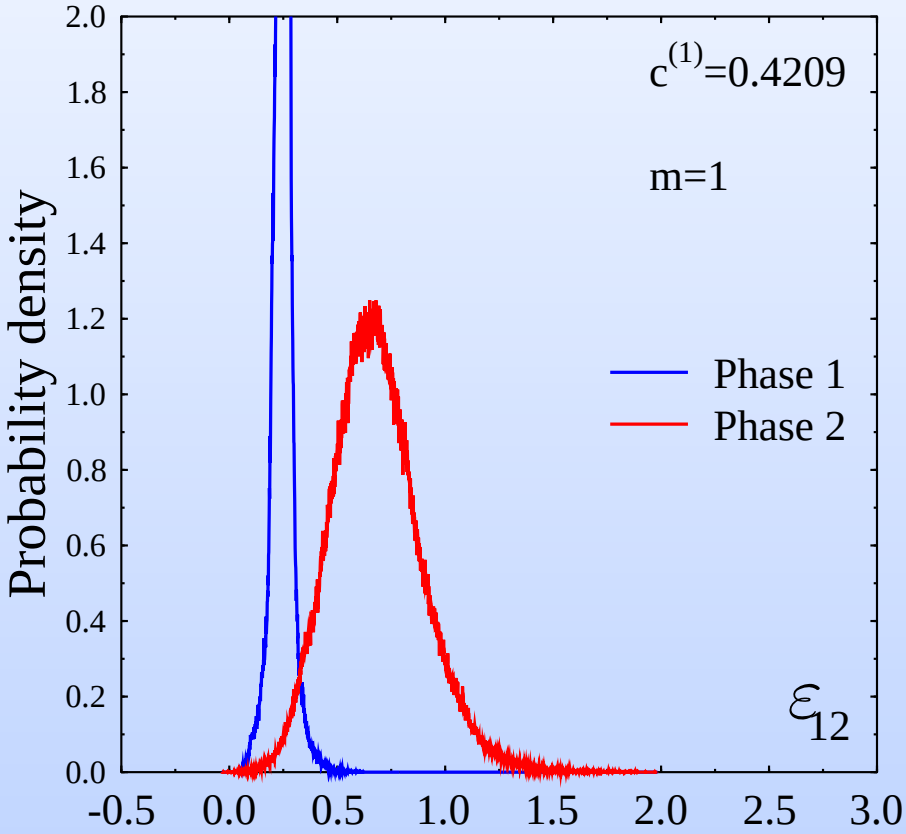
$n = 10$

Phase 1 (fibers) : $\overline{\varepsilon}^{(1)} \searrow$ **when** $n \nearrow$**.** Phase 2 (matrix) : **strain concentration (high fluctuations)** $\nearrow$ **when** $n \nearrow$**.**

Probability density

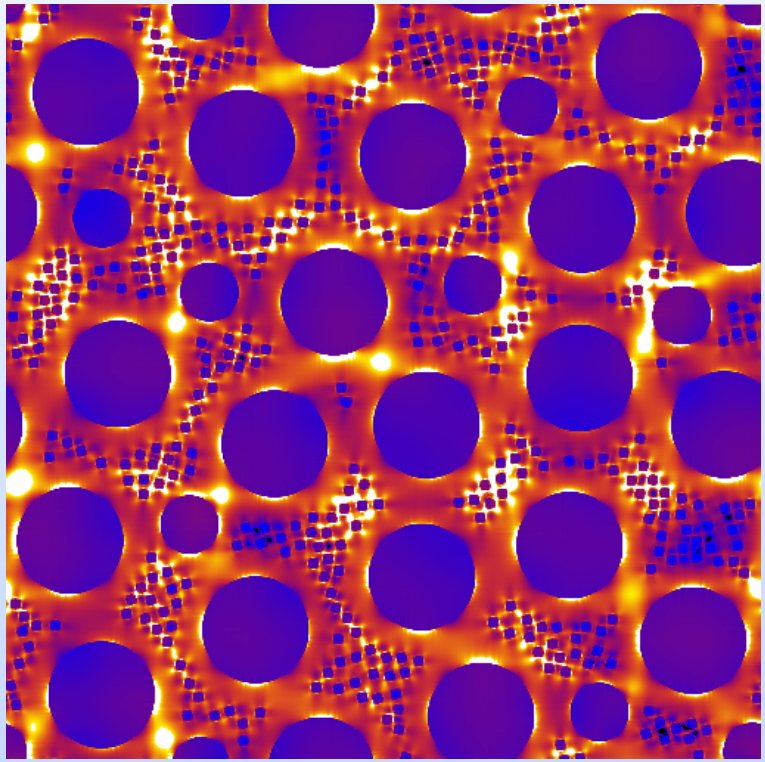
Snapshot and probability density for ε_{12}. $n = 1$.

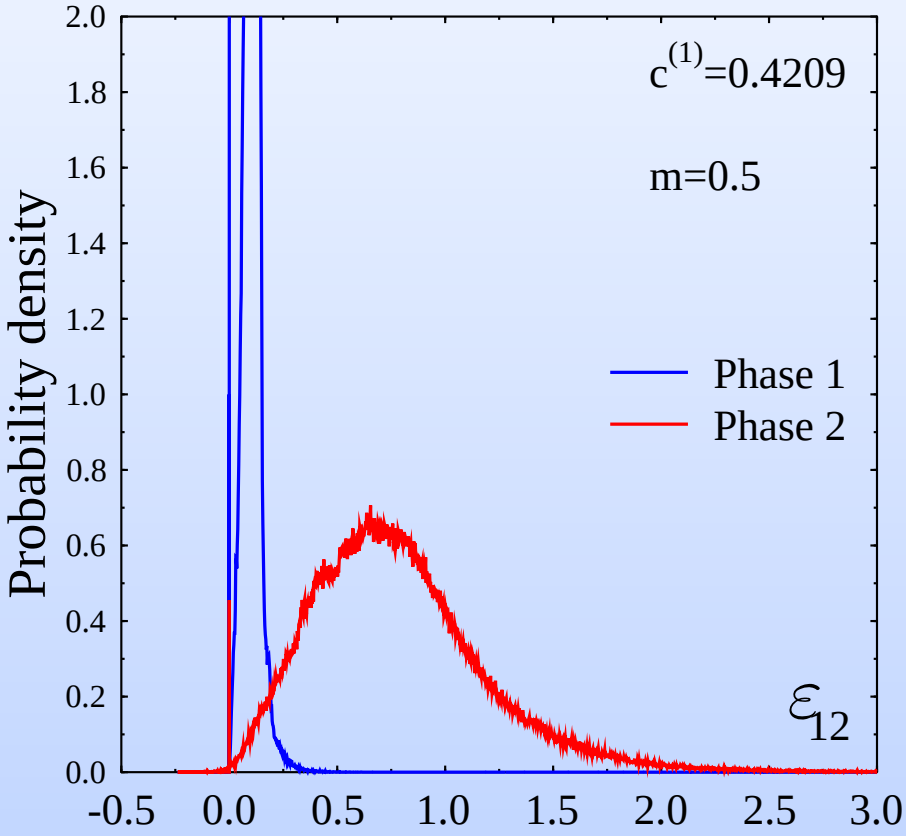




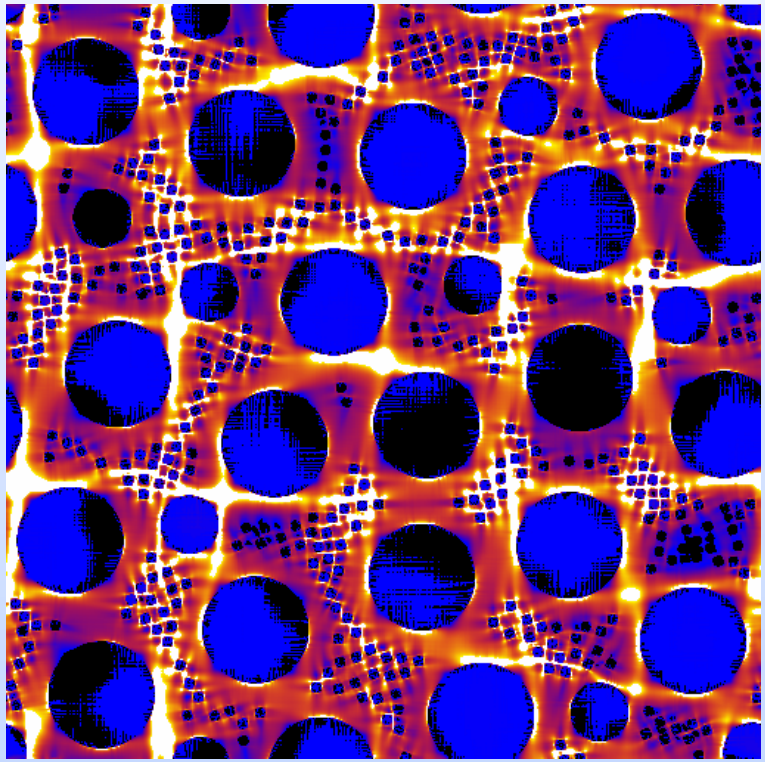
$n = 1$ **: the probability density can reasonably be considered as being Gaussian.**

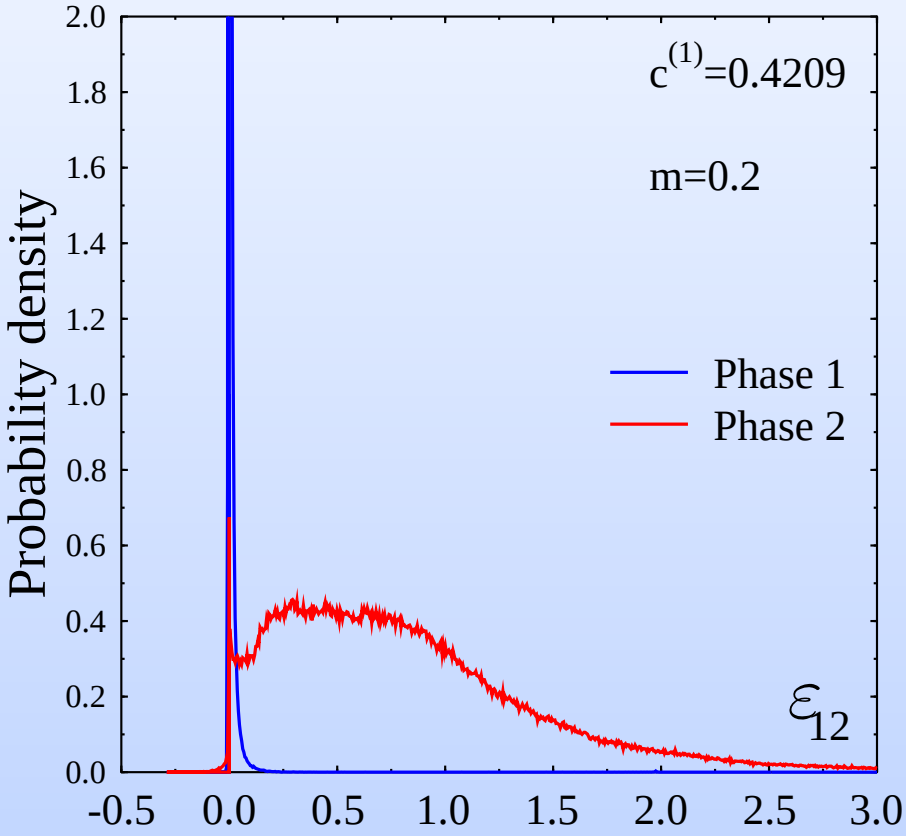
$n = 2$



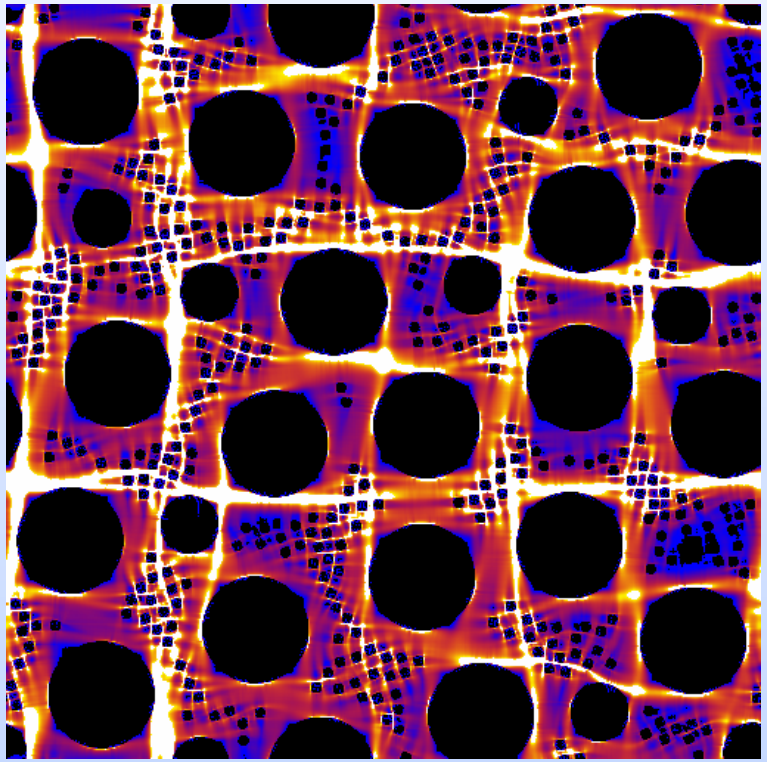

Probability density
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
c(1)=0.4209
m=0.5
Phase 1
Phase 2
ε12

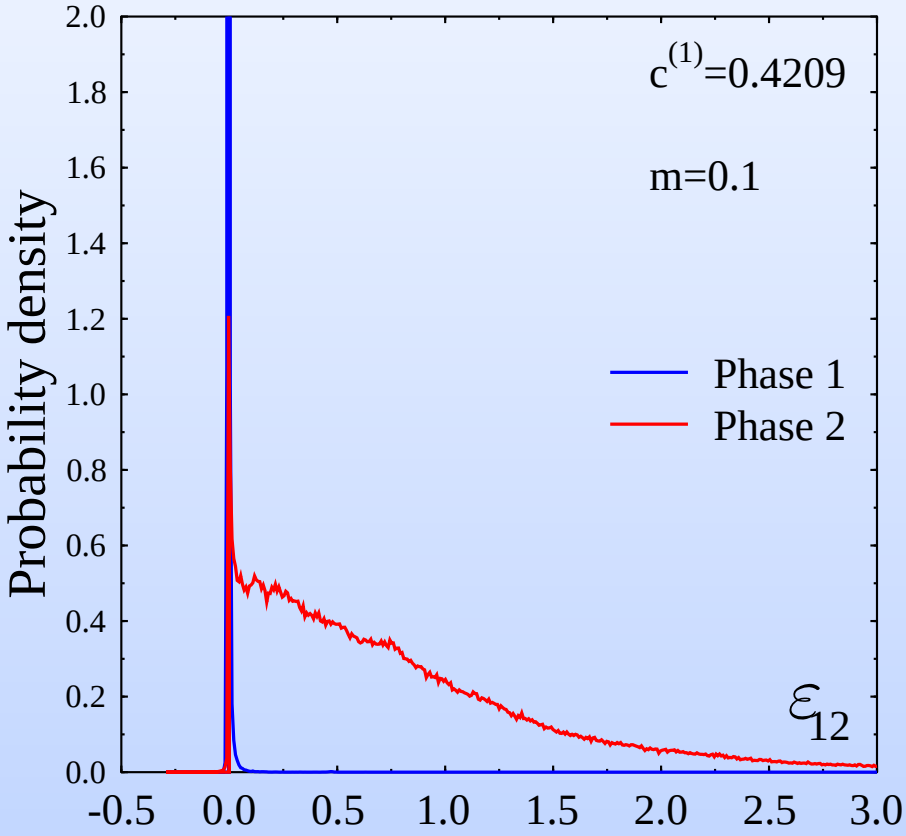
$n = 5$




Probability density
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
c(1)=0.4209
m=0.2
Phase 1
Phase 2
ε12

$n = 10$




Probability density
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
c(1)=0.4209
m=0.1
Phase 1
Phase 2
ε12

Comments

- Localized strains (which have a tremendous influence on the effective properties) correspond to the **tail** of the probability density. $\Rightarrow$ **higher order moments of the strain field should be accounted for.**
- These higher order moments are unknown in the actual nonlinear composite. **Only the first and second moments are known for linear composites (with random microstructure).**
- High fluctuations not well captured by the first moment. Introduce the second moment (Qiu and Weng, 1992, Buryachenko, 1993, Suquet, 1995, Hu, 1996) :

$$\left\langle \varepsilon_{\text{eq}}^2 \right\rangle_r = \frac{2}{3}\boldsymbol{K} :: \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_r, \quad \varepsilon_{\text{eff}}^{(r)} = (\left\langle \varepsilon_{\text{eq}}^2 \right\rangle_r)^{1/2}.$$

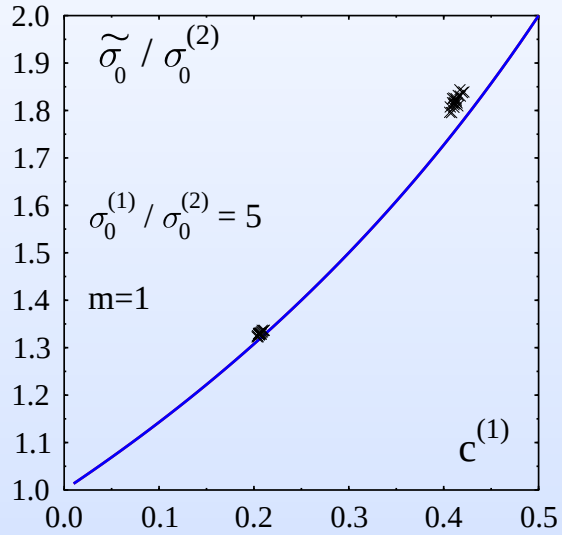
Second moment of the strain field in the LCC :

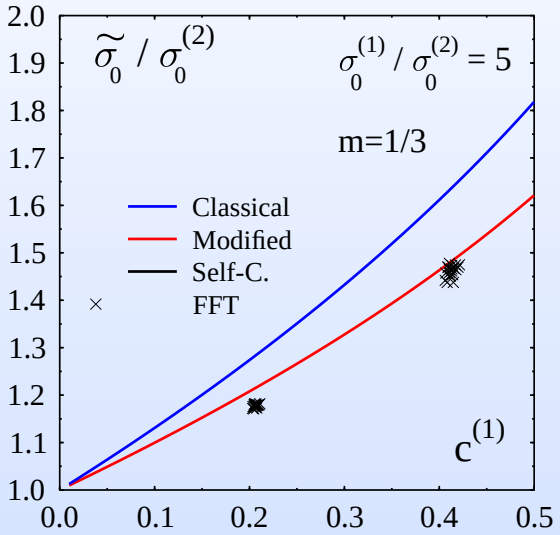
$$< \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} >_r = \frac{1}{c^{(r)}}\, \overline{\boldsymbol{\varepsilon}} : \frac{\partial \widetilde{\boldsymbol{L}}}{\partial \boldsymbol{L}^{(r)}} : \overline{\boldsymbol{\varepsilon}}, \quad \left\langle \varepsilon_{\text{eq}}^2 \right\rangle_r = \frac{1}{3c^{(r)}}\, \overline{\boldsymbol{\varepsilon}} : \frac{\partial \widetilde{\boldsymbol{L}}}{\partial \mu^{(r)}} : \overline{\boldsymbol{\varepsilon}}.$$

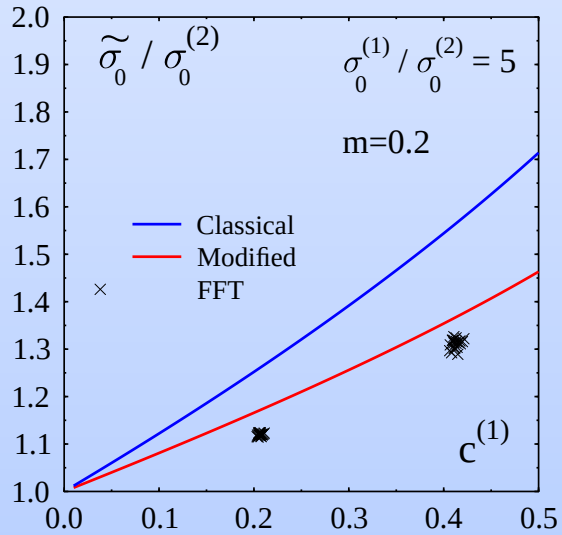
$\Rightarrow$ Modified secant theory based on the second moment of the strain.

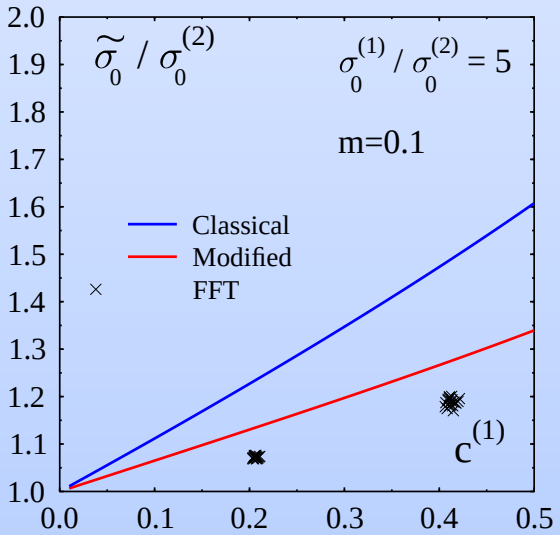
- It turns out (PS, 95) that the modified secant procedure **is equivalent** to the variational procedure of Ponte Castañeda ($\Rightarrow$ delivers an upper bound).

Effective flow-stress. The effective properties of the LCC are estimated by the lower Hashin-Shtrikman bound.



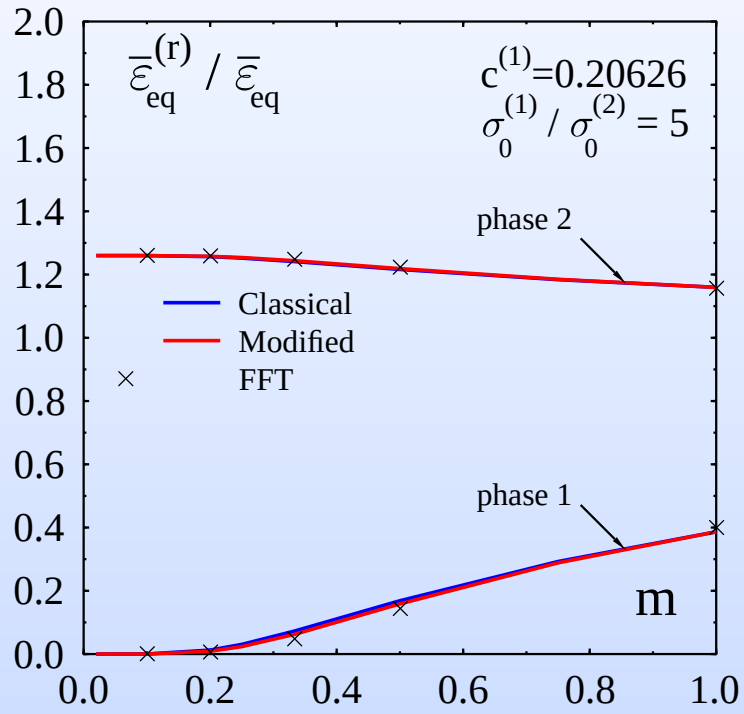


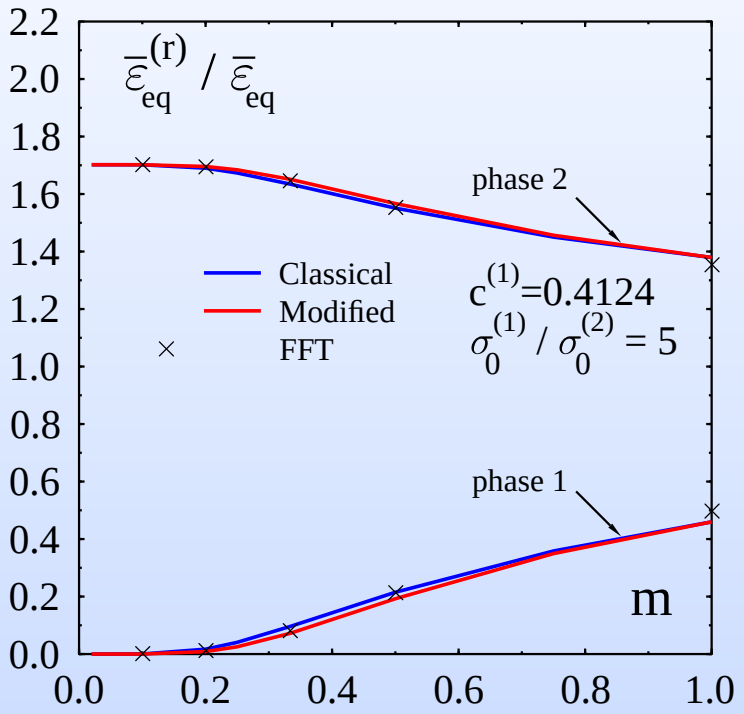




Classical = mean-field theory (1st moment), Modified = based on second-moments.

Average strain per phase (1st moment)



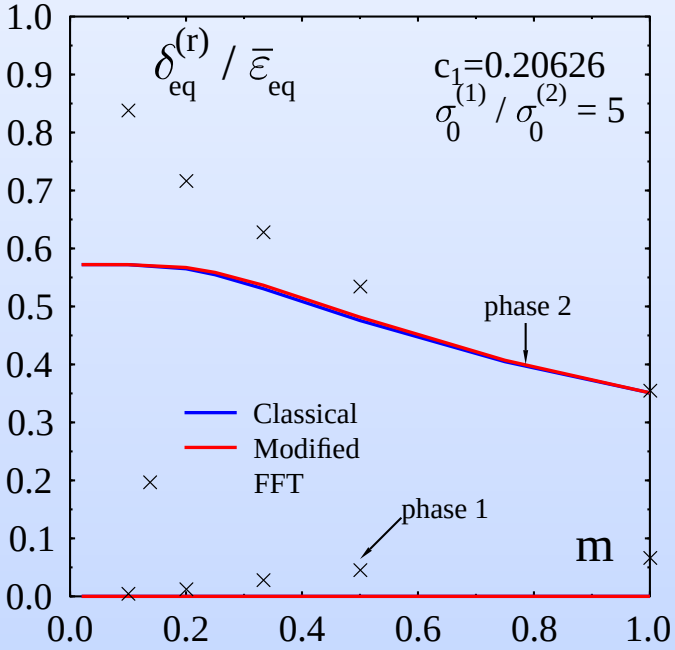


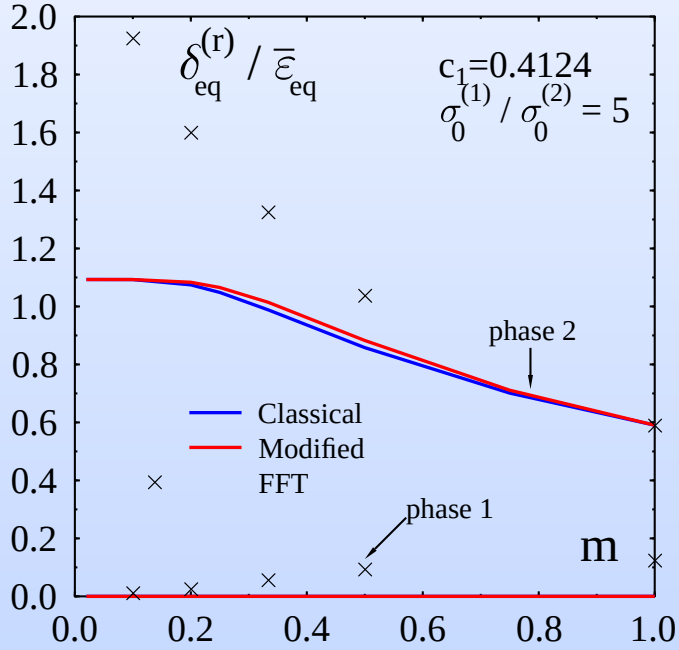
Stiff fibers, the average strain per phase is almost prescribed by the fiber volume fraction :

$$\varepsilon^{(2)} \simeq \frac{1}{c^{(2)}} \overline{\varepsilon}.$$

Quadratic fluctuations. Strain fluctuations in phase r : $\varepsilon - \overline{\varepsilon}^{(r)}$.

Isotropic invariant : $$\delta_{\text{eq}}^{(r)} = \left\langle \frac{2}{3}(\varepsilon_{ij} - \overline{\varepsilon}_{ij}^{(r)})(\varepsilon_{ij} - \overline{\varepsilon}_{ij}^{(r)}) \right\rangle_r^{1/2}.$$



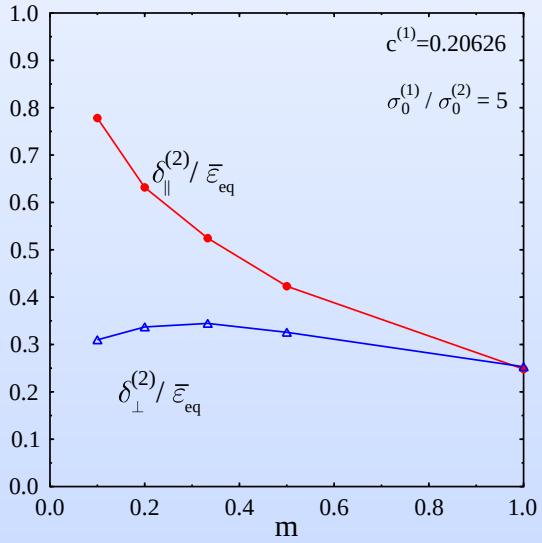


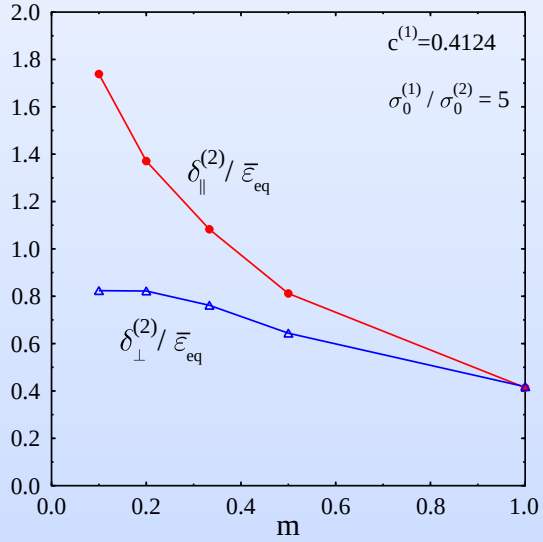
Fluctuations of the strain in the matrix $\nearrow$ when $m \searrow 0$. Blow-up not well captured by the secant theories.

Anisotropic measure of fluctuations (introduced by Ponte Castañeda, 2002)

$$\boldsymbol{C}_{\varepsilon}^{(r)} = \left\langle \boldsymbol{\varepsilon} - \overline{\boldsymbol{\varepsilon}}^{(r)} \otimes \boldsymbol{\varepsilon} - \overline{\boldsymbol{\varepsilon}}^{(r)} \right\rangle, \quad \boldsymbol{E}^{(r)} = \frac{2}{3}\frac{\overline{\boldsymbol{\varepsilon}}^{(r)}}{\overline{\varepsilon}_{\mathrm{eq}}^{(r)}} \otimes \frac{\overline{\boldsymbol{\varepsilon}}^{(r)}}{\overline{\varepsilon}_{\mathrm{eq}}^{(r)}}, \quad \boldsymbol{F}^{(r)} = \boldsymbol{K} - \boldsymbol{E}^{(r)}.$$

$$\delta_{||}^{(r)} = \sqrt{\frac{2}{3}\boldsymbol{E}^{(r)} :: \boldsymbol{C}_{\varepsilon}^{(r)}}, \quad \delta_{\perp}^{(r)} = \sqrt{\frac{2}{3}\boldsymbol{F}^{(r)} :: \boldsymbol{C}_{\varepsilon}^{(r)}}, \quad \delta_{\mathrm{eq}}^{(r)} = \sqrt{(\delta_{||}^{(r)})^2 + (\delta_{\perp}^{(r)})^2}.$$





- **Fluctuations are anisotropic**. Not taken into account by the secant theories (only by the recent “new second-order method” of Ponte Castañeda, 2002, 2004).
- At present **only second moment(s)** of the strain fluctuations are incorporated in analytical schemes. No analytical mean to compute higher order-moments.
- $\Rightarrow$ ***ad hoc* theories accounting for the nonuniformity of plastic strain fields.**

Concluding remarks

- **In nonlinear composites** intraphase field heterogeneity can be large. It has an important influence on the effective properties of composites.
- **Moments up to order 2** can be computed analytically. Higher order moments also contain essential information.
- The heterogeneity of the plastic strain field can be built in **approximate (but accurate) models** : **Nonuniform Transformation Field Analysis**.

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