A stochastic 3-scale method for polycrystalline materials

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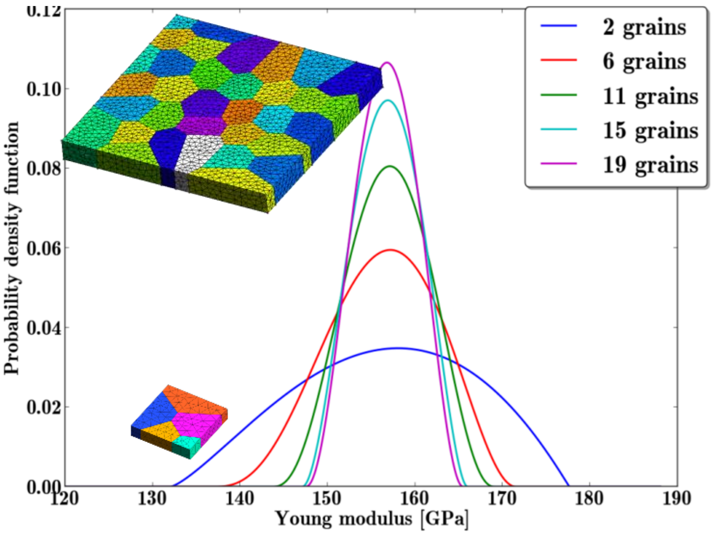
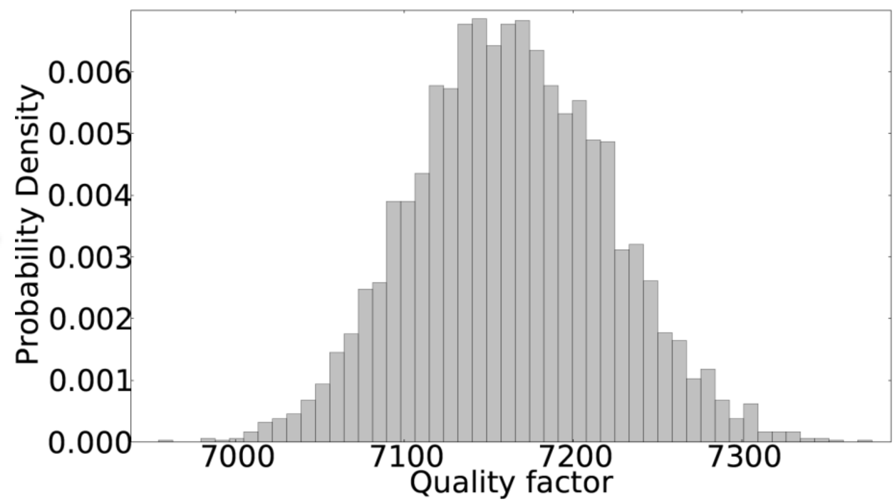
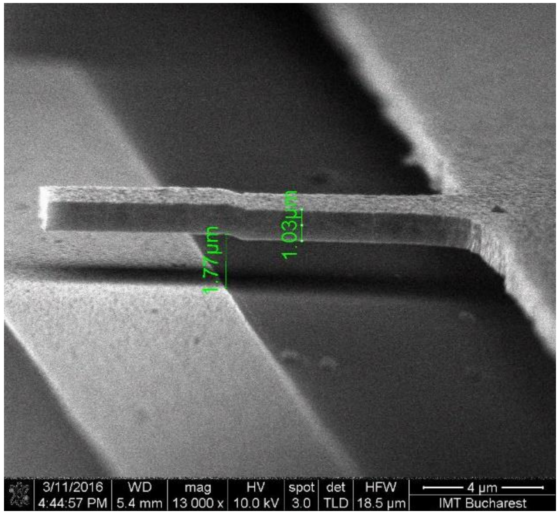




3SMVIB: The research has been funded by the Walloon Region under the agreement no 1117477 (CT-INT 2011-11-14) in the context of the ERA-NET MNT framework. Experimental measurements provided by IMT Bucharest (Voicu Rodica, Baracu Angela, Muller Raluca)

The problem



- MEMS structures
  - Are not several orders larger than their micro-structure size
  - Parameters-dependent manufacturing process
    - Low Pressure Chemical Vapor Deposition (LPCVD)
    - Properties depend on the temperature, time process, and flow gas conditions
  - Scatter in the structural properties
    - Due to the fabrication process (photolithography, etching …)
    - Due to uncertainties of the material
    - …

→ The objective of this work is to estimate this scatter

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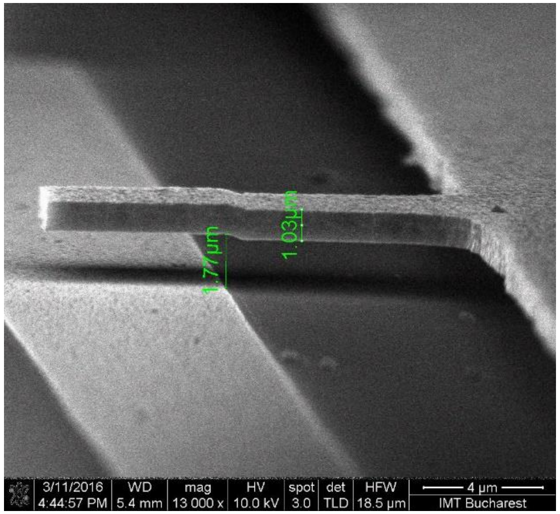
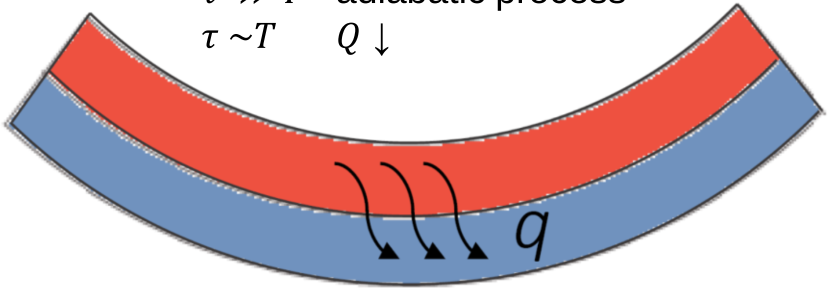


→ The objective of this work is to estimate this scatter

- Application example
  - Poly-silicon resonators
  - Quantities of interest
    - Eigen frequency
    - Quality factor due to thermo-elastic damping Q ~ $W/\Delta W$
    - Thermoelastic damping is a source of intrinsic material damping present in almost all materials

$\tau \ll T$ isothermal process
$\tau \gg T$ adiabatic process
$\tau \sim T$ $Q \downarrow$

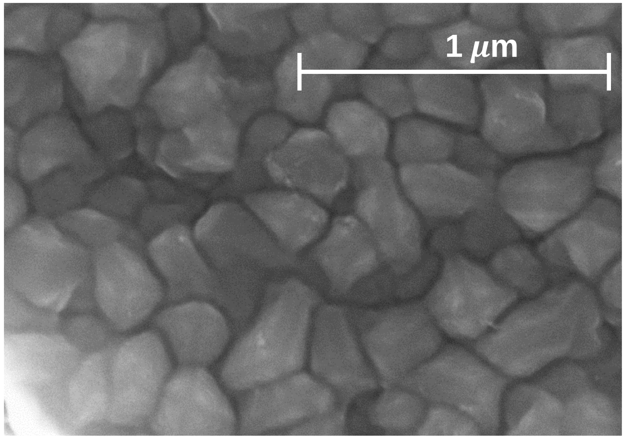


The problem

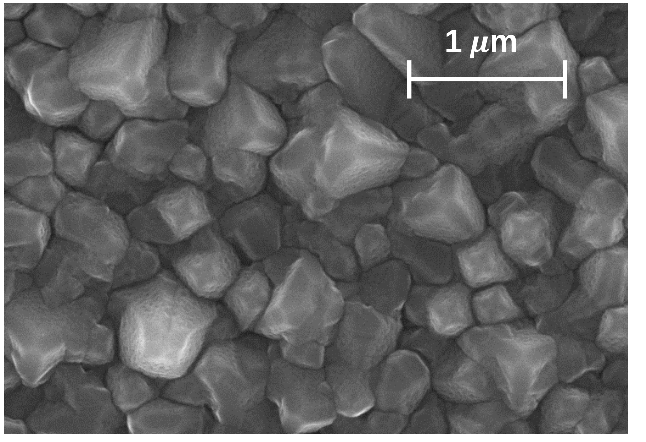
- Material structure: grain size distribution

  SEM Measurements (Scanning Electron Microscope)

  - Grain size dependent on the LPCVD temperature process
  - 2 µm-thick poly-silicon films



Deposition temperature: 580 °C



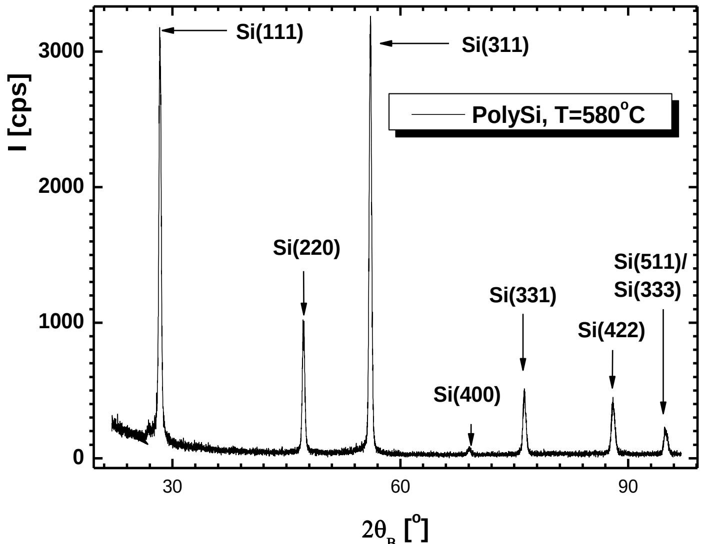
Deposition temperature: 650 °C

Deposition temperature [°C]	580	610	630	650
Average grain diameter [µm]	0.21	0.45	0.72	0.83

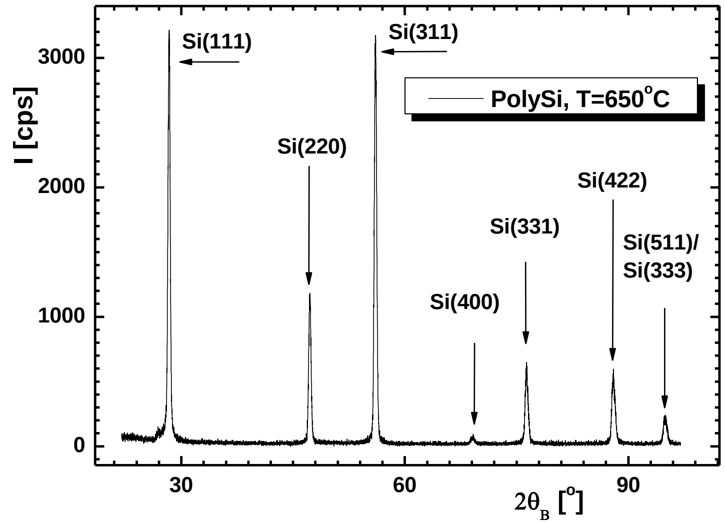
SEM images provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

The problem

- Material structure: grain orientation distribution
  - Grain orientation by XRD (X-ray Diffraction) measurements on 2 µm-thick poly-silicon films



Deposition temperature: 580 ºC



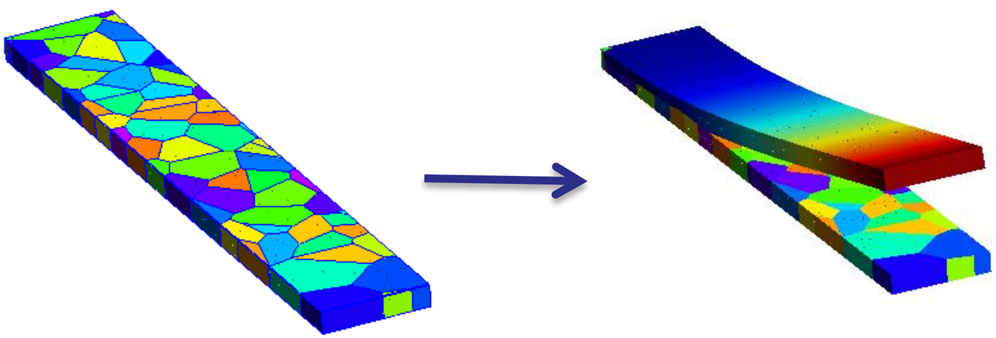
Deposition temperature: 630 ºC

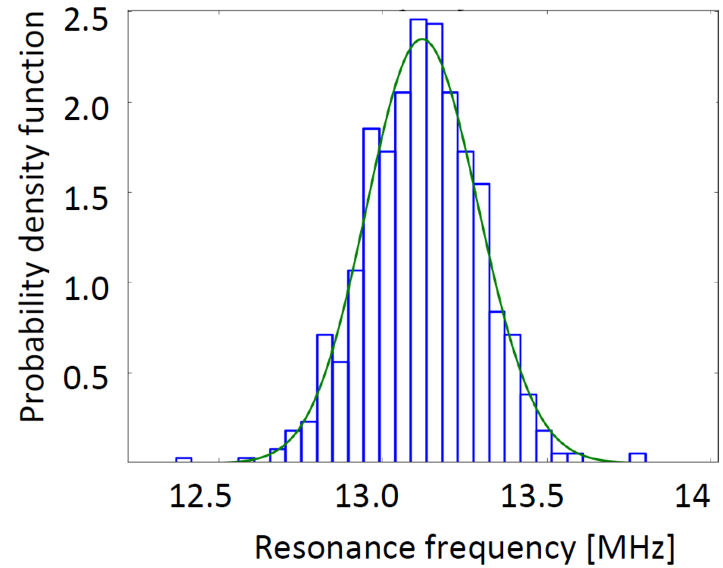
Deposition temperature [ºC]	580	610	630	650
<111> [%]	12.57	19.96	12.88	11.72
<220> [%]	7.19	13.67	7.96	7.59
<311> [%]	42.83	28.83	39.08	38.47
<400> [%]	4.28	5.54	3.13	3.93
<331> [%]	17.97	18.14	21.32	20.45
<422> [%]	15.15	13.86	15.63	17.84

XRD images provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

Monte-Carlo for a fully modelled beam

- The first mode frequency distribution can be obtained with
  - A 3D beam with each grain modelled
  - Grains distribution according to experimental measurements
  - Monte-Carlo simulations

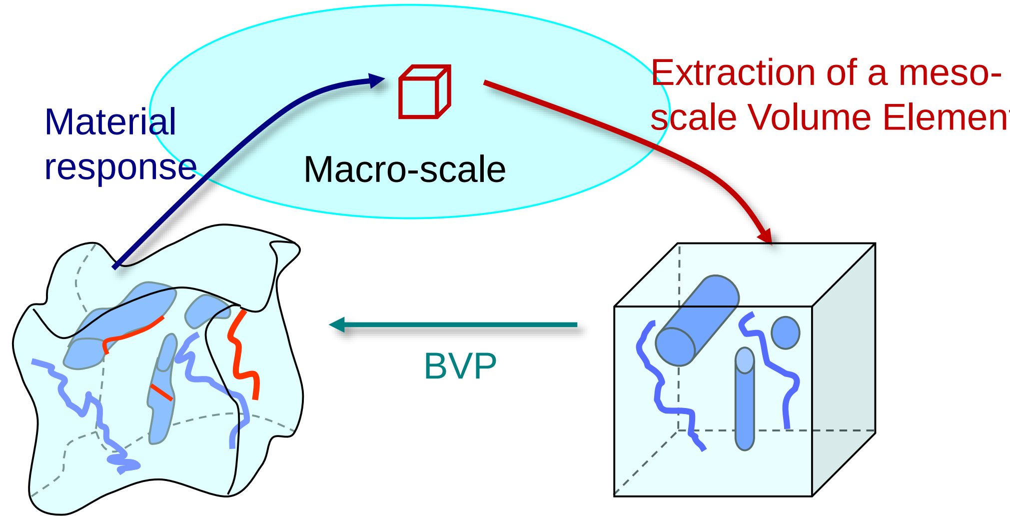




- Considering each grain is expensive and time consuming

  ↳ **Motivation for stochastic multi-scale methods**

- Multi-scale modelling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)



- Length-scales separation

$$L_{macro} >> L_{VE} >> L_{micro}$$

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

To be statistically representative: Size of the meso-scale volume element larger than the characteristic length of the micro-structure

Motivations

- For structures not several orders larger than the micro-structure size

$$L_{macro} >> L_{VE} >\sim L_{micro}$$

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

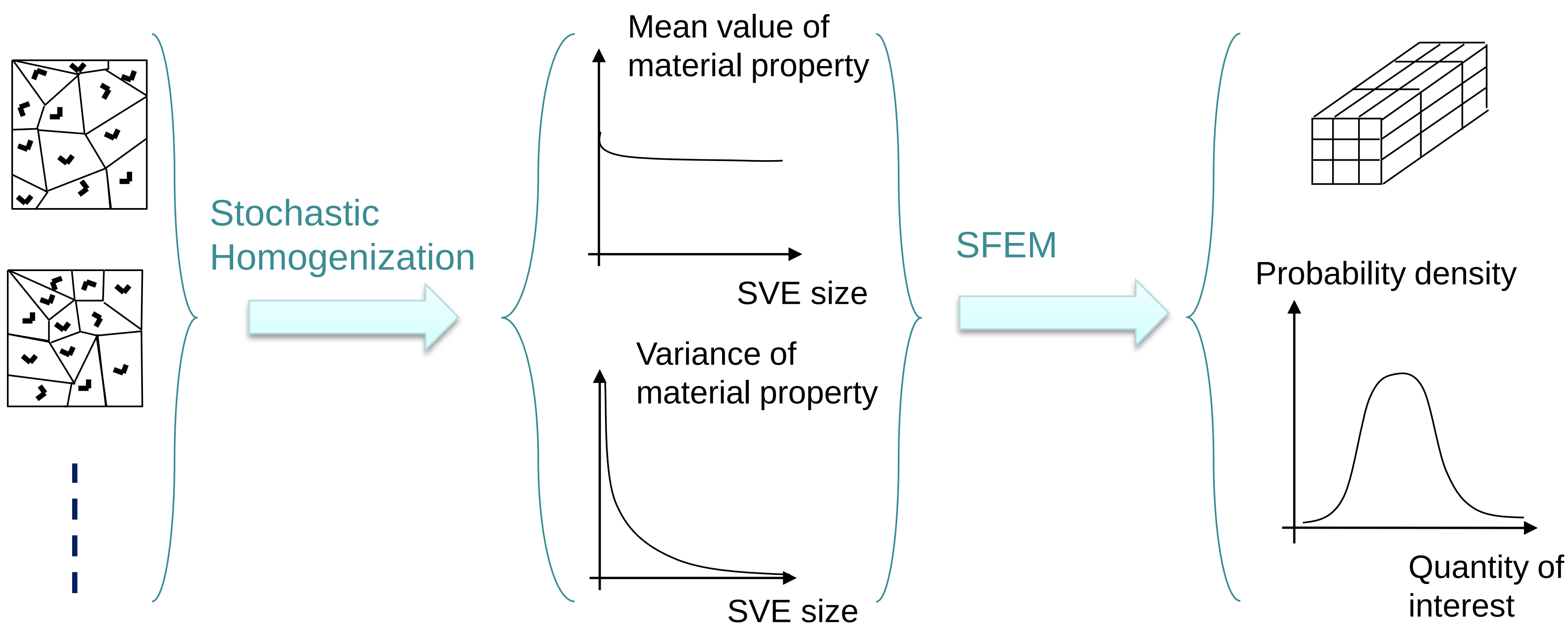
Meso-scale volume element no longer statistically representative: Stochastic Volume Elements*

- Possibility to propagate the uncertainties from the micro-scale to the macro-scale

**M Ostoja-Starzewski, X Wang, 1999*
P Trovalusci, M Ostoja-Starzewski, M L De Bellis, A Murrali, 2015
X. Yin, W. Chen, A. To, C. McVeigh, 2008
J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem, 2011
….

A 3-scale process

Grain-scale or micro-scale	Meso-scale	Macro-scale
➢ Samples of the microstructure (volume elements) are generated ➢ Each grain has a random orientation	➢ Intermediate scale ➢ The distribution of the material property $\mathbb{P}(C)$ is defined	➢ Uncertainty quantification of the macro-scale quantity ➢ E.g. the first mode frequency $\mathbb{P}(f_1)$ /Quality factor $\mathbb{P}(Q)$



Content

- From the micro-scale to the meso-scale
  - Thermo-mechanical homogenization
  - Definition of Stochastic Volume Elements (SVEs) & Stochastic homogenization
  - Need for a meso-scale random field
- The meso-scale random field
  - Definition of the thermo-mechanical meso-scale random field
  - Stochastic model of the random field: Spectral generator & non-Gaussian mapping
- From the meso-scale to the macro-scale
  - 3-Scale approach verification
  - Application to extract the quality factor
- Accounting for roughness effect
  - From the micro-scale to the meso-scale
  - The meso-scale random field
  - From the meso-scale to the macro-scale

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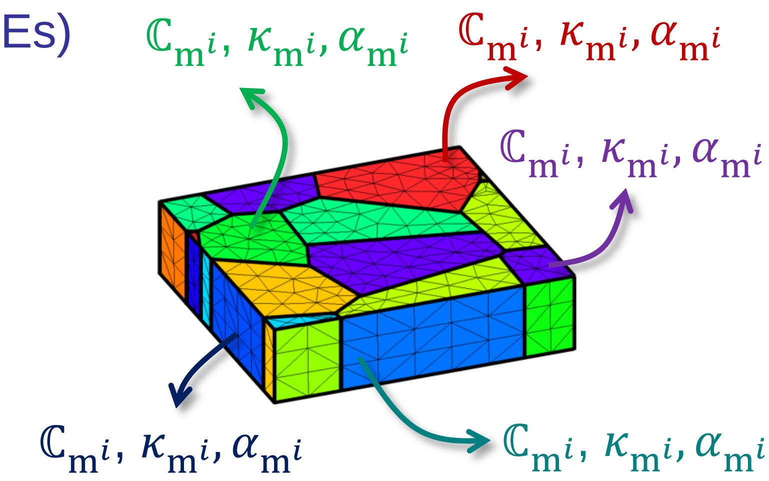
From the micro-scale to the meso-scale

- Definition of Stochastic Volume Elements (SVEs)
  - Poisson Voronoï tessellation realizations
    - SVE realization ω_j
  - Each grain ω_i is assigned material properties
    - Elasticity tensor $\mathbb{C}_{\mathrm{m}^i}$;
    - Heat conductivity tensor κ_{m^i} ;
    - Thermal expansion tensors α_{m^i} .
    - Defined from silicon crystal properties
  - Each set $\mathbb{C}_{m^i}, \kappa_{\mathrm{m}^i}, \alpha_{\mathrm{m}^i}$ is assigned a random orientation
    - Following XRD distributions



$\omega_j = \cup_i \, \omega_i$

- Stochastic homogenization
  - Several SVE realizations
  - For each SVE $\omega_j = \cup_i \, \omega_i$

$$\mathbb{C}_{\mathrm{m}^i}, \kappa_{\mathrm{m}^i}, \alpha_{\mathrm{m}^i} \quad \forall i \longrightarrow \mathbb{C}_{\mathrm{M}^j}, \kappa_{\mathrm{M}^j}, \alpha_{\mathrm{M}^j}$$

Computational homogenization

Samples of the meso-scale homogenized elasticity tensors

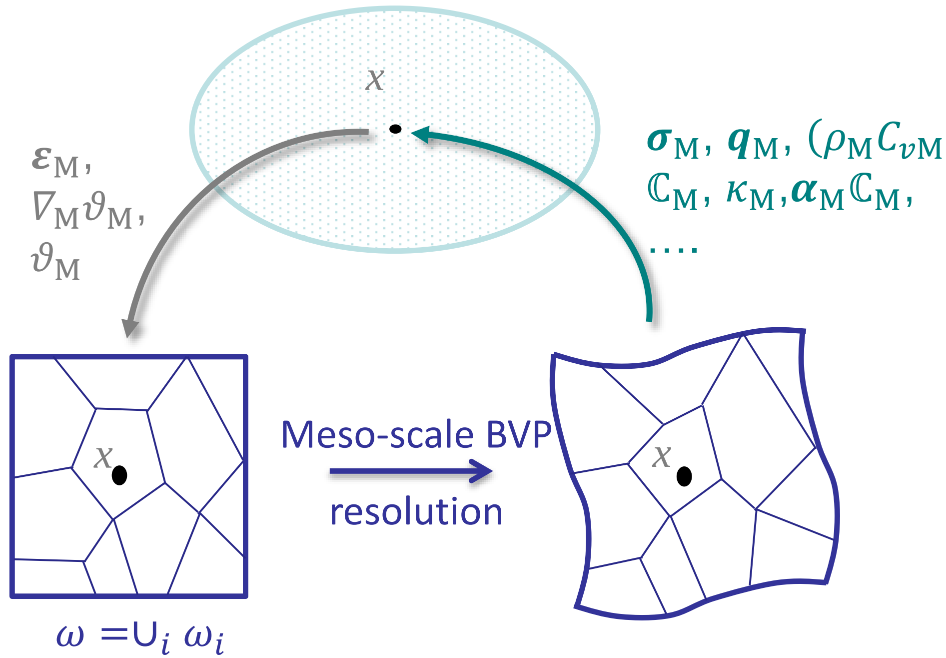
  - Homogenized material tensors not unique as statistical representativeness is lost*

*"C. Huet, 1990

From the micro-scale to the meso-scale

- Thermo-mechanical homogenization
  - Down-scaling

$$\begin{cases} \boldsymbol{\varepsilon}_{\mathrm{M}} = \dfrac{1}{V(\omega)}\displaystyle\int_{\omega} \boldsymbol{\varepsilon}_{\mathrm{m}} d\omega \\ \nabla_{\mathrm{M}}\vartheta_{\mathrm{M}} = \dfrac{1}{V(\omega)}\displaystyle\int_{\omega} \nabla_{\mathrm{m}}\vartheta_{\mathrm{m}} d\omega \\ \vartheta_{\mathrm{M}} = \dfrac{1}{V(\omega)}\displaystyle\int_{\omega} \dfrac{\rho_{\mathrm{m}} C_{v\mathrm{m}}}{\rho_{\mathrm{M}} C_{v\mathrm{M}}} \vartheta_{\mathrm{m}} d\omega \end{cases}$$



  - Up-scaling

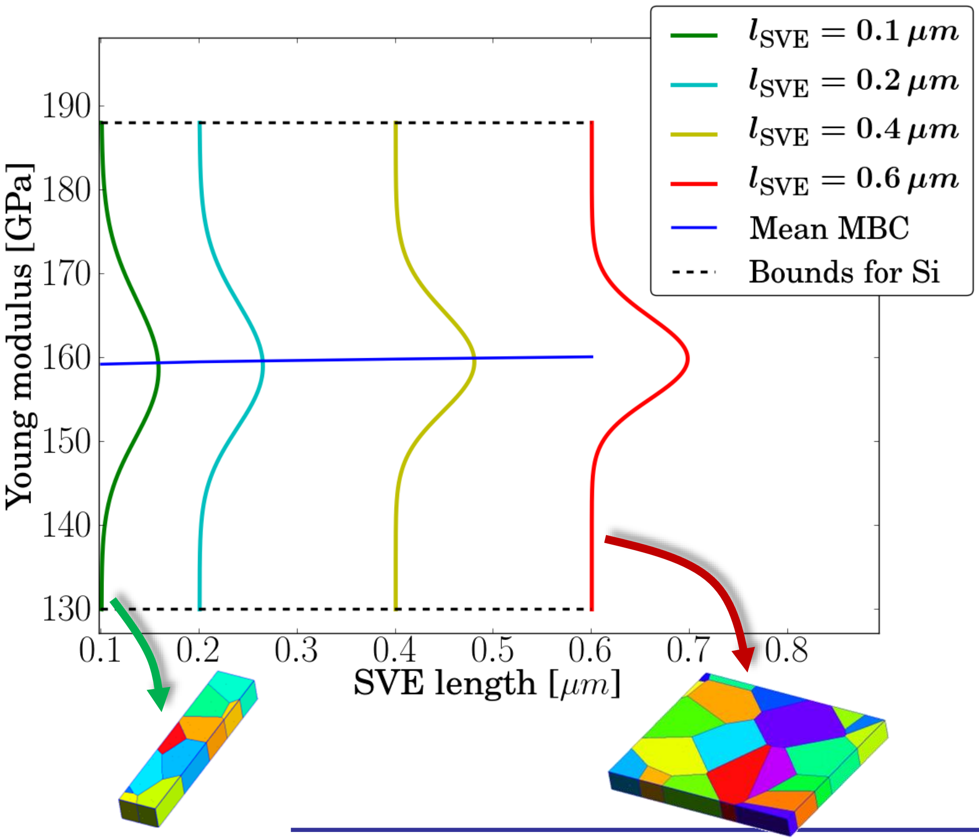
$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \dfrac{1}{V(\omega)}\displaystyle\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} d\omega \\ \boldsymbol{q}_{\mathrm{M}} = \dfrac{1}{V(\omega)}\displaystyle\int_{\omega} \boldsymbol{q}_{\mathrm{m}} d\omega \\ \rho_{\mathrm{M}} C_{v\mathrm{M}} = \dfrac{1}{V(\omega)}\displaystyle\int \rho_{\mathrm{m}} C_{v\mathrm{m}} dV \end{cases} \longrightarrow \begin{cases} \mathbb{C}_{\mathrm{M}} = \dfrac{\partial \boldsymbol{\sigma}_{\mathrm{M}}}{\partial \boldsymbol{u}_{\mathrm{M}} \otimes \boldsymbol{\nabla}_{\mathrm{M}}} \quad \& \quad \boldsymbol{\alpha}_{\mathrm{M}} : \mathbb{C}_{\mathrm{M}} = -\dfrac{\partial \boldsymbol{\sigma}_{\mathrm{M}}}{\partial \vartheta_{\mathrm{M}}} \\ \boldsymbol{\kappa}_{\mathrm{M}} = -\dfrac{\partial \boldsymbol{q}_{\mathrm{M}}}{\partial \nabla_{\mathrm{M}}\vartheta_{\mathrm{M}}} \end{cases}$$

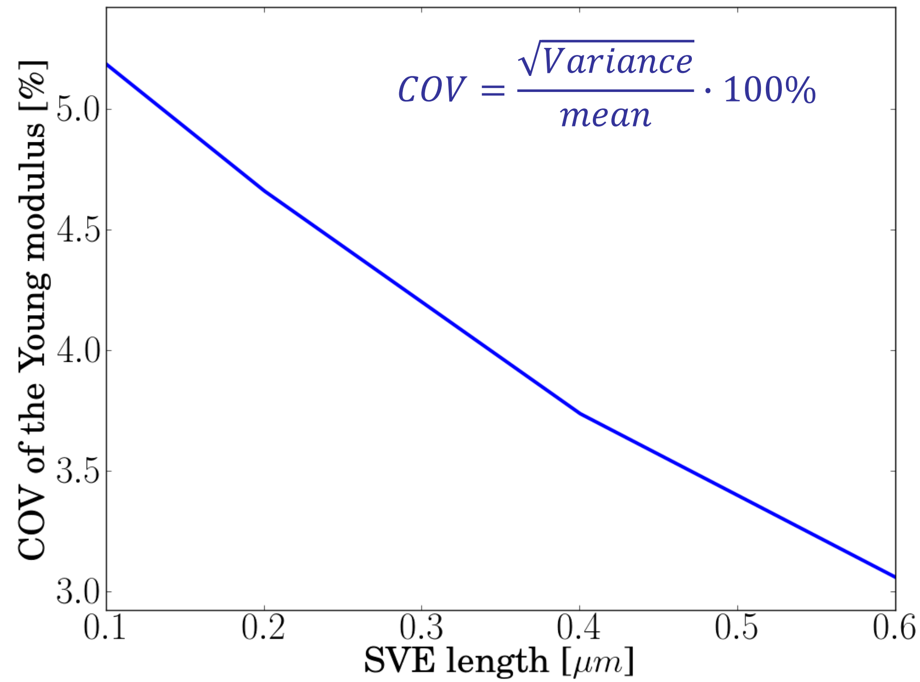
  - Consistency $\longrightarrow$ Satisfied by periodic boundary conditions

From the micro-scale to the meso-scale

- Distribution of the apparent meso-scale elasticity tensor $\mathbb{C}_M$

  - For large SVEs, the apparent tensor tends to the effective (and unique) one

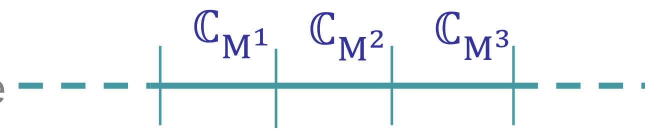


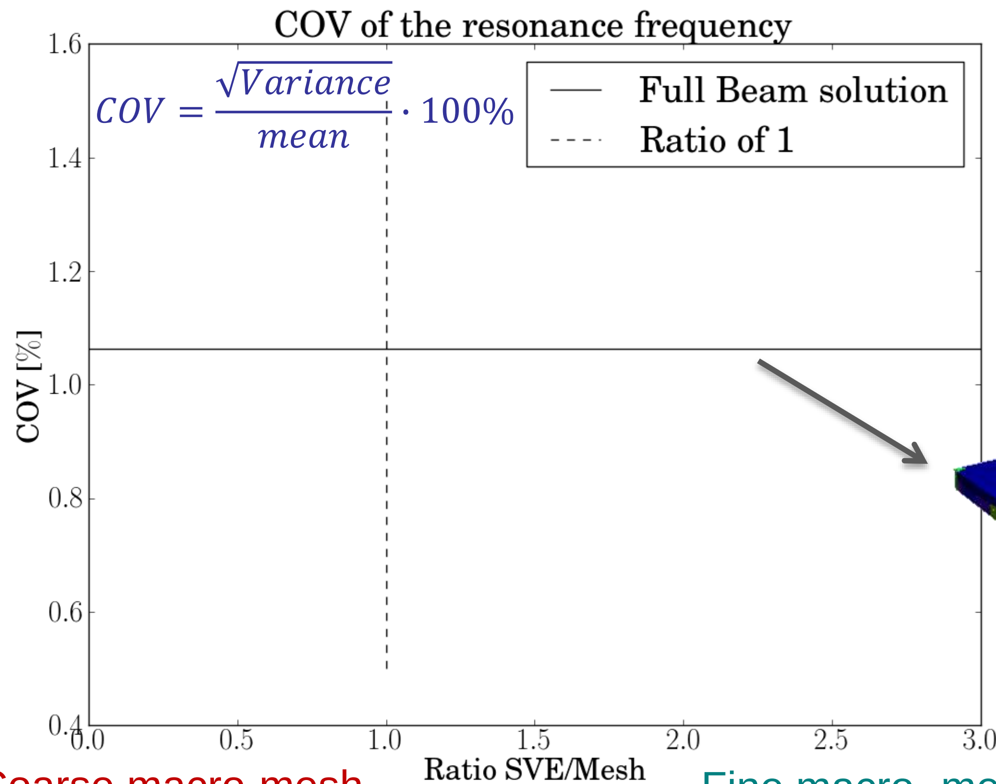


  - The bounds do not depend on the SVE size but on the silicon elasticity tensor

  - However, the larger the SVE, the lower the probability to be close to the bounds

- Use of the meso-scale distribution with macro-scale finite elements
  - Beam macro-scale finite elements
  - Use of the meso-scale distribution as a random variable
  - Monte-Carlo simulations



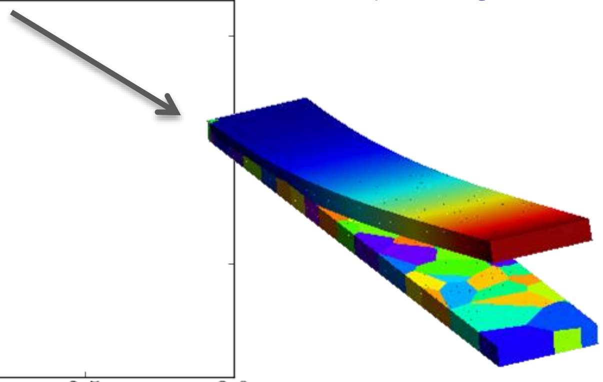


Coarse macro-mesh

Fine macro- mesh

First bending mode of

a 3.2 μm-long beam



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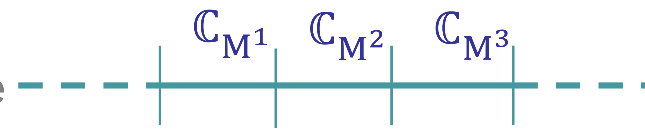
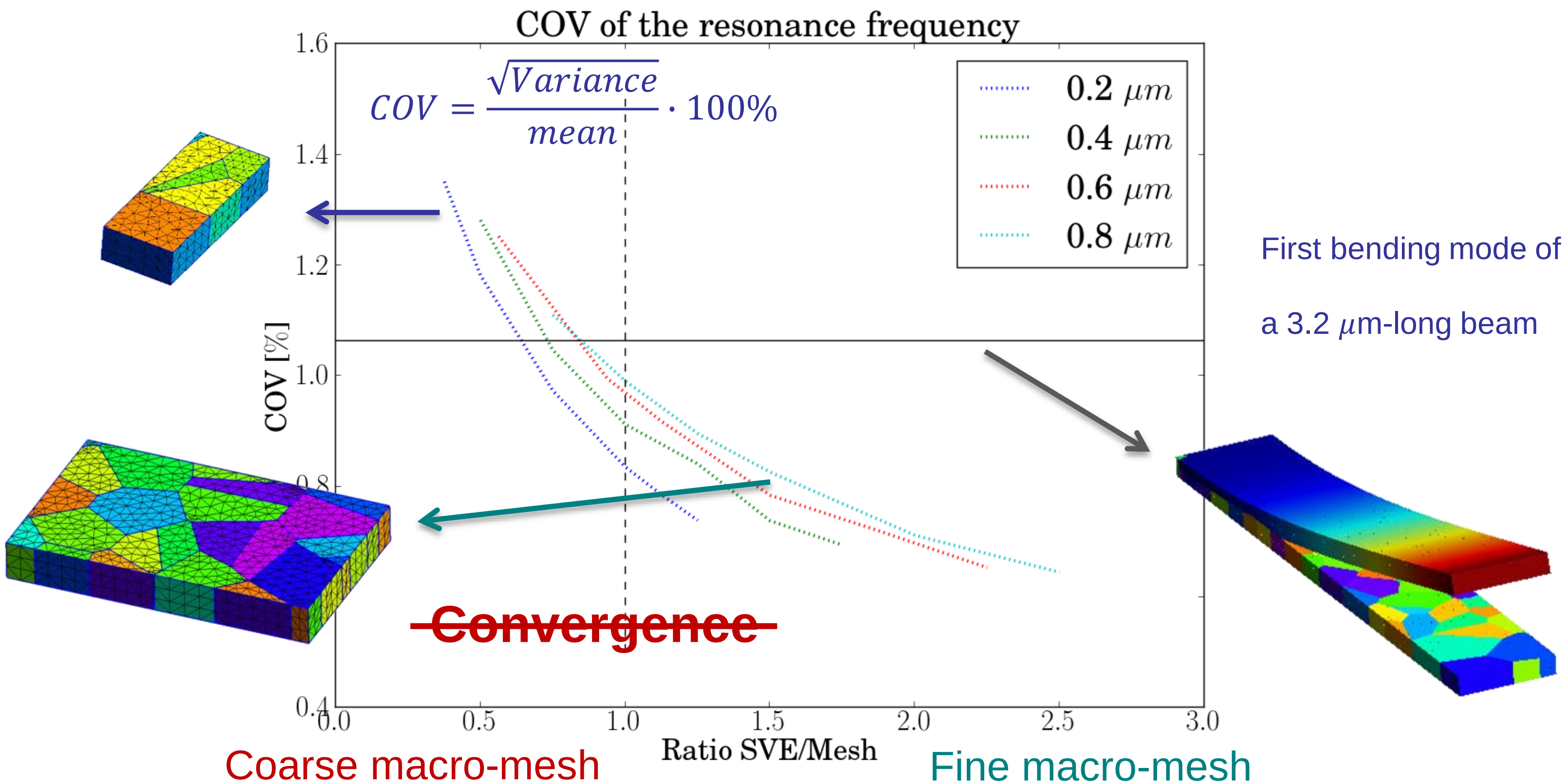
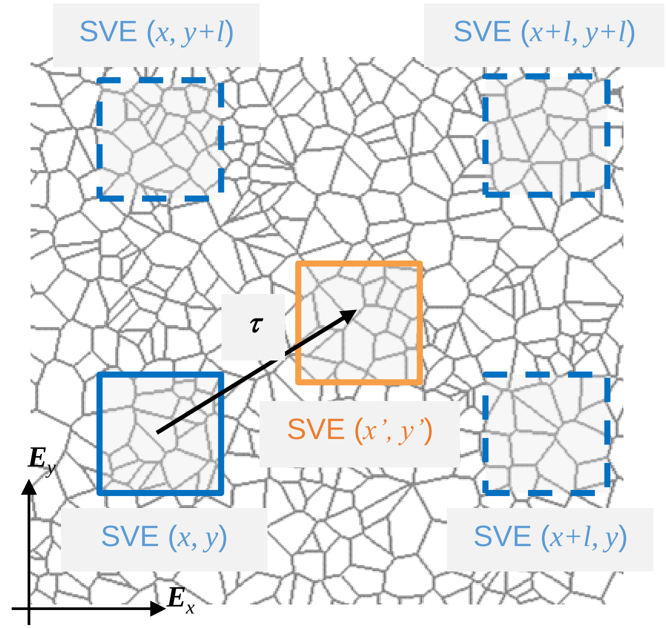




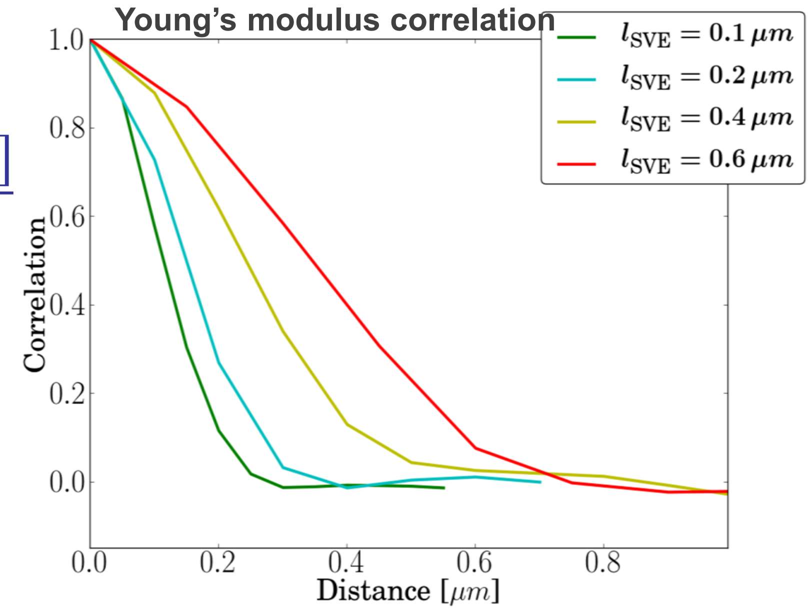
- No convergence: the macro-scale distribution (first resonance frequency) depends on SVE and mesh sizes

From the micro-scale to the meso-scale

- Need for a meso-scale random field
  - Introduction of the (meso-scale) spatial correlation
    - Define large tessellations
    - SVEs extracted at different distances in each tessellation
  - Evaluate the spatial correlation between the components of the meso-scale material operators
  - For example, in 1D-elasticity
    - Young's modulus correlation



$$R_{E_x}(\tau) = \frac{\mathbb{E}\left[\left(E_x(x) - \mathbb{E}(E_x)\right)\left(E_x(x+\tau) - \mathbb{E}(E_x)\right)\right]}{\mathbb{E}\left[\left(E_x - \mathbb{E}(E_x)\right)^2\right]}$$



    - Correlation length

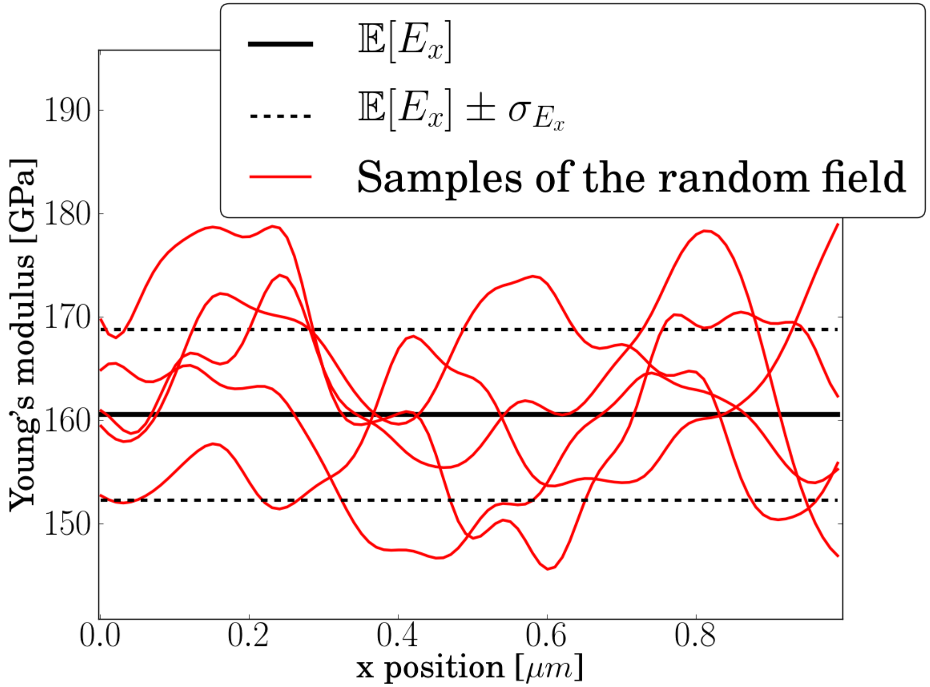
$$L_{E_x} = \frac{\int_{-\infty}^{\infty} R_{E_x}(\tau)d\tau}{R_{E_x}(0)}$$

From the micro-scale to the meso-scale

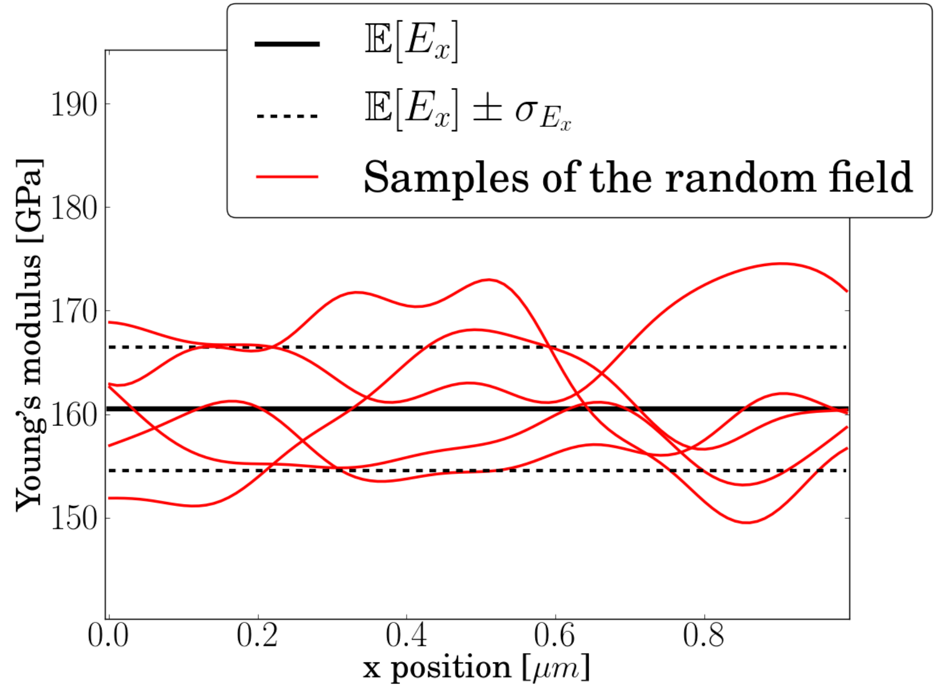
- Need for a meso-scale random field (2)
  - The meso-scale random field is characterized by the correlation length L_{E_x}
  - The correlation length L_{E_x} depends on the SVE size

Random field with different SVEs sizes

$l_{\text{SVE}} = 0.1\ \mu m$



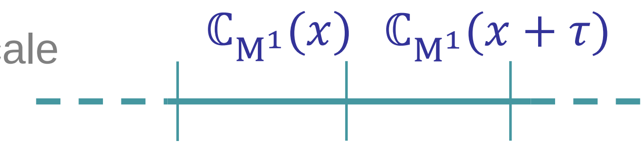
$l_{\text{SVE}} = 0.4\ \mu m$



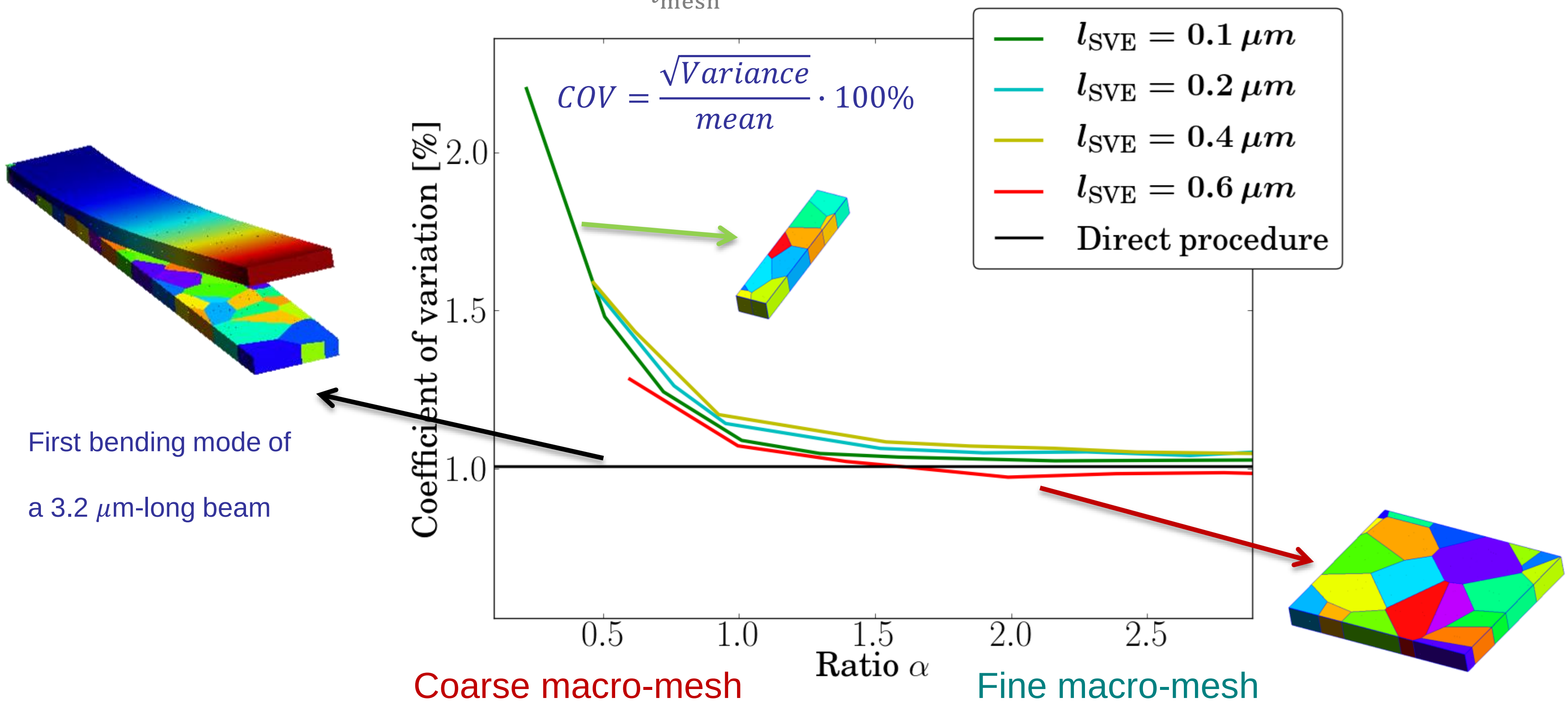
From the micro-scale to the meso-scale

- Need for a meso-scale random field (3)
  - Use of the meso-scale random field

    → Monte-Carlo simulations at the macro-scale

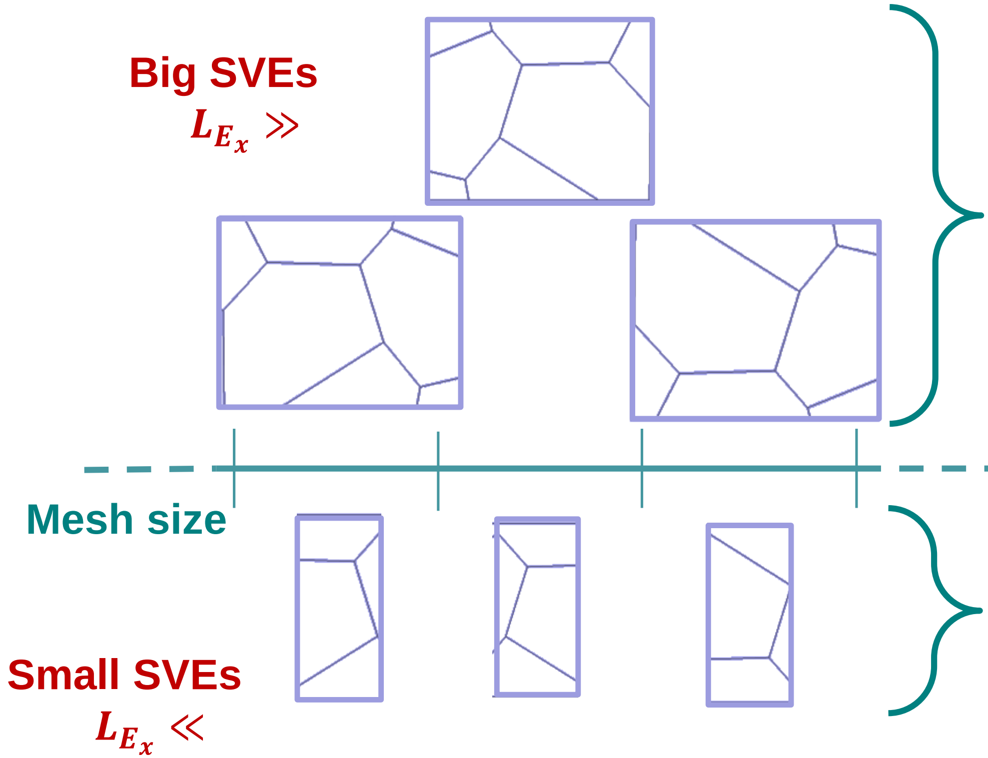


  - Macro-scale beam elements of size l_{mesh}
  - Convergence in terms of $\alpha = \frac{L_{E_x}}{l_{\text{mesh}}}$



From the micro-scale to the meso-scale

- Need for a meso-scale random field (3)
  - Effect of the ratio $\alpha = \frac{L_{E_x}}{l_{\text{mesh}}}$ (Only one gauss point in one element)



$\alpha = \frac{L_{E_x}}{l_{\text{mesh}}} > 1$ → The spatial correlation is accounted for

$\alpha = \frac{L_{E_x}}{l_{\text{mesh}}} < 1$ → For the spatial correlation to be accounted for, we need more integration points

  - For extreme values of α:
    - $\alpha \gg 1$: no more scale separation if $l_{\text{SVE}} \sim L_{\text{macro}}$
    - $\alpha \ll 1$: loss of microstructural details if $l_{\text{SVE}} \sim L_{\text{micro}}$

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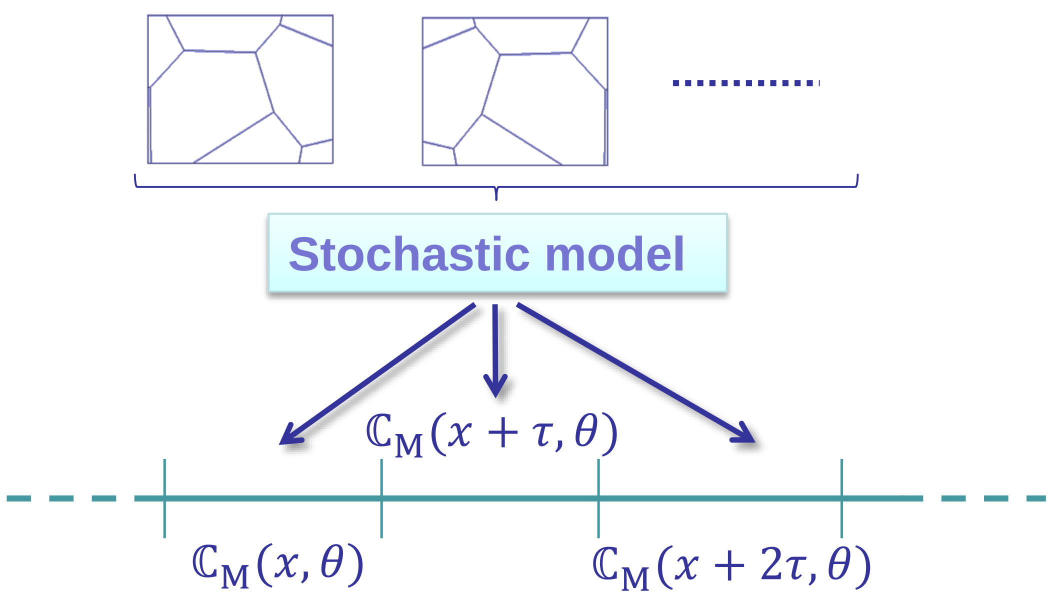
The meso-scale random field

- Use of the meso-scale distribution with stochastic (macro-scale) finite elements
  - Use of the meso-scale random field

    ⟶ Monte-Carlo simulations at the macro-scale

  - BUT we do not want to evaluate the random field from the stochastic homogenization for each simulation ⟶ Meso-scale random field from a generator

    ⟶ Need for a stochastic model of meso-scale elasticity tensors



The meso-scale random field

- Definition of the thermo-mechanical meso-scale random field
  - Elasticity tensor $\mathbb{C}_{\mathrm{M}}(x, \theta)$ (matrix form $\boldsymbol{C}_M$) & thermal conductivity $\boldsymbol{\kappa}_{\mathrm{M}}$ are bounded
    - Ensure existence of their inverse
    - Define lower bounds $\mathbb{C}_{\mathrm{L}}$ and $\boldsymbol{\kappa}_{\mathrm{L}}$ such that

$$\begin{cases} \boldsymbol{\varepsilon} : (\mathbb{C}_{\mathrm{M}} - \mathbb{C}_{\mathrm{L}}) : \boldsymbol{\varepsilon} > 0 & \forall \boldsymbol{\varepsilon} \\ \nabla\vartheta \cdot (\boldsymbol{\kappa}_{\mathrm{M}} - \boldsymbol{\kappa}_{\mathrm{L}}) \cdot \nabla\vartheta > 0 & \forall \nabla\vartheta \end{cases}$$

  - Use a Cholesky decomposition when semi-positive definite matrices are required

$$\begin{cases} \boldsymbol{C}_{\mathrm{M}}(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{C}_{\mathrm{L}} + \left(\overline{\boldsymbol{\mathcal{A}}} + \boldsymbol{\mathcal{A}}'(\boldsymbol{x}, \boldsymbol{\theta})\right)^T \left(\overline{\boldsymbol{\mathcal{A}}} + \boldsymbol{\mathcal{A}}'(\boldsymbol{x}, \boldsymbol{\theta})\right) \\ \boldsymbol{\kappa}_{\mathrm{M}}(\boldsymbol{x}, \boldsymbol{\theta}) = \boldsymbol{\kappa}_{\mathrm{L}} + \left(\overline{\boldsymbol{\mathcal{B}}} + \boldsymbol{\mathcal{B}}'(\boldsymbol{x}, \boldsymbol{\theta})\right)^T \left(\overline{\boldsymbol{\mathcal{B}}} + \boldsymbol{\mathcal{B}}'(\boldsymbol{x}, \boldsymbol{\theta})\right) \\ \boldsymbol{\alpha}_{\mathrm{M}_{ij}}(\boldsymbol{x}, \boldsymbol{\theta}) = \overline{\boldsymbol{\mathcal{V}}}^{(t)} + \boldsymbol{\mathcal{V}}'^{(t)}(\boldsymbol{x}, \boldsymbol{\theta}) \end{cases}$$

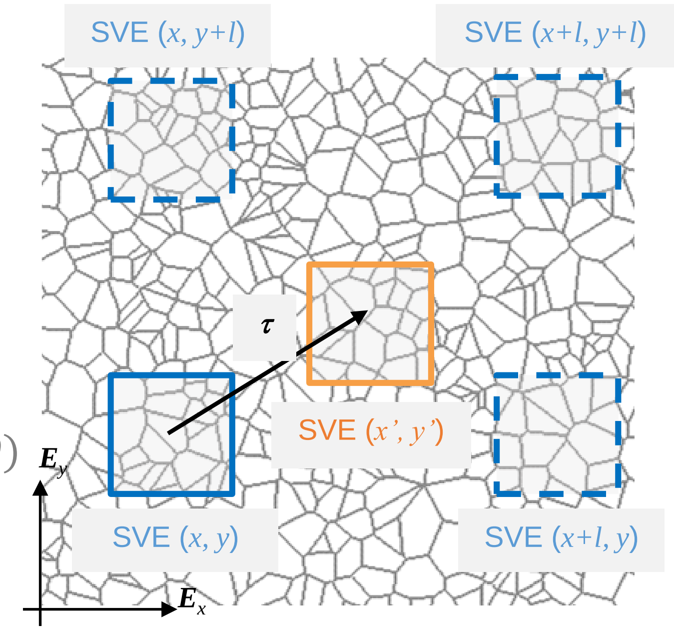
  - We define the homogenous zero-mean random field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x}, \boldsymbol{\theta})$, with as entries
    - Elasticity tensor $\mathcal{A}'(\boldsymbol{x}, \boldsymbol{\theta}) \Rightarrow \boldsymbol{\mathcal{V}}'^{(1)}$ … $\boldsymbol{\mathcal{V}}'^{(21)}$,
    - Heat conductivity tensor $\mathcal{B}'(\boldsymbol{x}, \boldsymbol{\theta}) \Rightarrow \boldsymbol{\mathcal{V}}'^{(22)}$ … $\boldsymbol{\mathcal{V}}'^{(27)}$
    - Thermal expansion tensors $\boldsymbol{\mathcal{V}}'^{(t)} \Rightarrow \boldsymbol{\mathcal{V}}'^{(28)}$ … $\boldsymbol{\mathcal{V}}'^{(33)}$

The meso-scale random field

- Characterization of the meso-scale random field
  - Generate large tessellation realizations
  - For each tessellation realization
    - Extract SVEs centered on $\boldsymbol{x} + \boldsymbol{\tau}$
    - For each SVE evaluate $\mathbb{C}_{\mathrm{M}}(\boldsymbol{x} + \boldsymbol{\tau})$, $\kappa_{\mathrm{M}}(\boldsymbol{x} + \boldsymbol{\tau}), \alpha_{\mathrm{M}}(\boldsymbol{x} + \boldsymbol{\tau})$
  - From the set of realizations $\mathbb{C}_{\mathrm{M}}(\boldsymbol{x}, \boldsymbol{\theta})$, $\kappa_{\mathrm{M}}(\boldsymbol{x}, \boldsymbol{\theta}), \alpha_{\mathrm{M}}(\boldsymbol{x}, \boldsymbol{\theta})$
    - Evaluate the bounds $\mathbb{C}_{\mathrm{L}}$ and $\boldsymbol{\kappa}_{\mathrm{L}}$
    - Apply the Cholesky decomposition $\Rightarrow$ $\boldsymbol{\mathcal{A}}'(\boldsymbol{x}, \boldsymbol{\theta})$, $\boldsymbol{\mathcal{B}}'(\boldsymbol{x}, \boldsymbol{\theta})$
    - Fill the 33 entries of the zero-mean homogenous field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x}, \boldsymbol{\theta})$
  - Compute the auto-/cross-correlation matrix

$$R_{\boldsymbol{\mathcal{V}}'}^{(rs)}(\boldsymbol{\tau}) = \frac{\mathbb{E}\left[\boldsymbol{\mathcal{V}}'^{(r)}(\boldsymbol{x})\boldsymbol{\mathcal{V}}'^{(s)}(\boldsymbol{x} + \boldsymbol{\tau})\right]}{\sqrt{\mathbb{E}[(\boldsymbol{\mathcal{V}}'^{(r)})^2]\mathbb{E}[(\boldsymbol{\mathcal{V}}'^{(s)})^2]}}$$

  - Generate zero-mean random field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x}, \boldsymbol{\theta})$
    - Spectral generator & non-Gaussian mapping



The meso-scale random field

- Stochastic model of the meso-scale random field: Spectral generator*
  - Start from the auto-/cross-covariance matrix

$$\tilde{R}^{(rs)}_{\boldsymbol{\mathcal{V}}'}(\boldsymbol{\tau}) = \sigma_{\boldsymbol{\mathcal{V}}'^{(r)}}\sigma_{\boldsymbol{\mathcal{V}}'^{(s)}} R^{(rs)}_{\boldsymbol{\mathcal{V}}'}(\boldsymbol{\tau}) = \mathbb{E}\left[\left(\boldsymbol{\mathcal{V}}'^{(r)}(\boldsymbol{x}) - \mathbb{E}\left(\boldsymbol{\mathcal{V}}'^{(r)}\right)\right)\left(\boldsymbol{\mathcal{V}}'^{(s)}(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}\left(\boldsymbol{\mathcal{V}}'^{(s)}\right)\right)\right]$$

  - Evaluate the spectral density matrix from the periodized zero-padded matrix $\widetilde{\boldsymbol{R}}^{\mathrm{P}}_{\boldsymbol{\mathcal{V}}'}(\boldsymbol{\tau})$

$$\boldsymbol{S}^{(rs)}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right] = \sum_{n} \widetilde{R}^{\mathrm{P}\ (rs)}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\tau}^{(\boldsymbol{n})}\right] e^{-2\pi i \boldsymbol{\tau}^{(n)}\cdot\boldsymbol{\omega}^{(\boldsymbol{m})}} \quad \& \quad \boldsymbol{S}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right] = \boldsymbol{H}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]\boldsymbol{H}^{*}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]$$

    - $\boldsymbol{\omega}$ gathers the discrete frequencies
    - $\boldsymbol{\tau}$ gathers the discrete spatial locations
  - Generate a Gaussian random field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x}, \boldsymbol{\theta})$

$$\boldsymbol{\mathcal{V}}'^{(r)}(\boldsymbol{x},\boldsymbol{\theta}) = \sqrt{2\Delta\omega}\,\Re\left(\sum_{s}\sum_{\boldsymbol{m}} \boldsymbol{H}^{(\boldsymbol{rs})}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]\eta^{(s,\boldsymbol{m})}\, e^{2\pi i\left(\boldsymbol{x}\cdot\boldsymbol{\omega}^{(\boldsymbol{m})}+\boldsymbol{\theta}^{(s,\boldsymbol{m})}\right)}\right)$$

    - $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$ are independent random variables
  - Quid if a non-Gaussian distribution is sought?

Shinozuka, M., Deodatis, G., 1988

The meso-scale random field

- Stochastic model of the meso-scale random field: non-Gaussian mapping*
  - Start from micro-sampling of the stochastic homogenization
    - The continuous form of the targeted PSD function

$$\boldsymbol{S}^{\mathrm{T}^{(rs)}}(\boldsymbol{\omega}) = \Delta\boldsymbol{\tau}\boldsymbol{S}_{\boldsymbol{\mathcal{V}}'}^{(rs)}\left[\boldsymbol{\omega}^{(m)}\right] = \Delta\boldsymbol{\tau}\sum_{n}\widetilde{R}_{\boldsymbol{\mathcal{V}}'}^{\mathrm{P}\,(rs)}\left[\boldsymbol{\tau}^{(n)}\right]e^{-2\pi i\boldsymbol{\tau}^{(n)}\cdot\boldsymbol{\omega}^{(m)}}$$

    - The targeted marginal distribution density function $\boldsymbol{F}^{\mathrm{NG}(\boldsymbol{r})}$ of the random variable $\boldsymbol{\mathcal{V}}'^{(\boldsymbol{r})}$
    - A marginal Gaussian distribution $\boldsymbol{F}^{G(\boldsymbol{r})}$ of zero-mean and targeted variance $\boldsymbol{\sigma}_{\boldsymbol{\mathcal{V}}'^{(r)}}$
  - Iterate

Generate Gaussian random vector $\boldsymbol{\mathcal{V}}'^{\mathrm{G}}(\boldsymbol{x})$ from $\boldsymbol{S}^{(rs)}(\boldsymbol{\omega})$

Map $\boldsymbol{\mathcal{V}}'^{G}(\boldsymbol{x})$ to a non-Gaussian field:
$$\boldsymbol{\mathcal{V}}'^{\mathrm{NG}^{(r)}}(\boldsymbol{x}) = \boldsymbol{F}^{\mathrm{NG}(\boldsymbol{r})^{-1}}\left(\boldsymbol{F}^{\mathrm{G}(\boldsymbol{r})}\left(\boldsymbol{\mathcal{V}}'^{\mathrm{G}^{(r)}}(\boldsymbol{x})\right)\right)$$

Evaluate the PSD $\boldsymbol{S}^{\mathrm{NG}^{(rs)}}(\boldsymbol{\omega})$ of $\boldsymbol{\mathcal{V}}'^{\mathrm{NG}}(\boldsymbol{x})$

$\boldsymbol{S}^{\mathrm{NG}^{(rs)}} \simeq \boldsymbol{S}^{\mathrm{T}^{(rs)}}$?

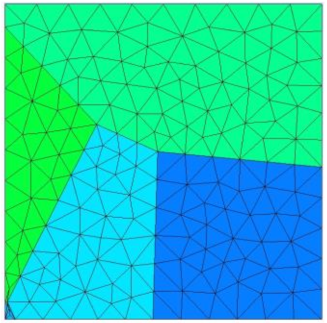
No

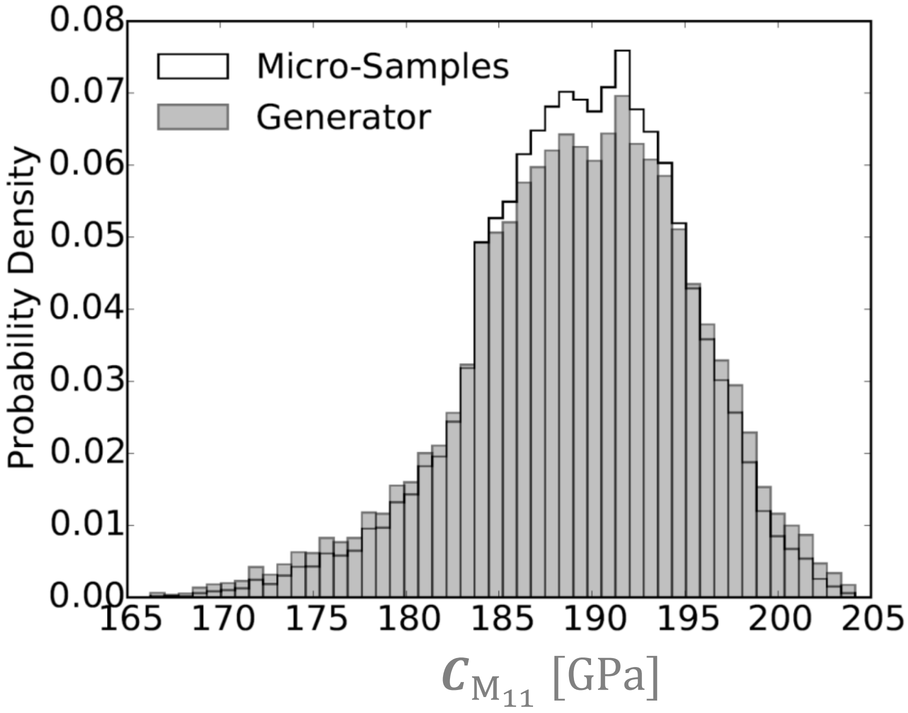
$$\boldsymbol{S}^{(rs)}(\boldsymbol{\omega}) \leftarrow \boldsymbol{S}^{(rs)}(\boldsymbol{\omega})\frac{\boldsymbol{S}^{\mathrm{T}^{(rr)}}(\boldsymbol{\omega})\boldsymbol{S}^{\mathrm{T}^{(ss)}}(\boldsymbol{\omega})}{\boldsymbol{S}^{\mathrm{NG}^{(rr)}}(\boldsymbol{\omega})\boldsymbol{S}^{\mathrm{NG}^{(ss)}}(\boldsymbol{\omega})}$$

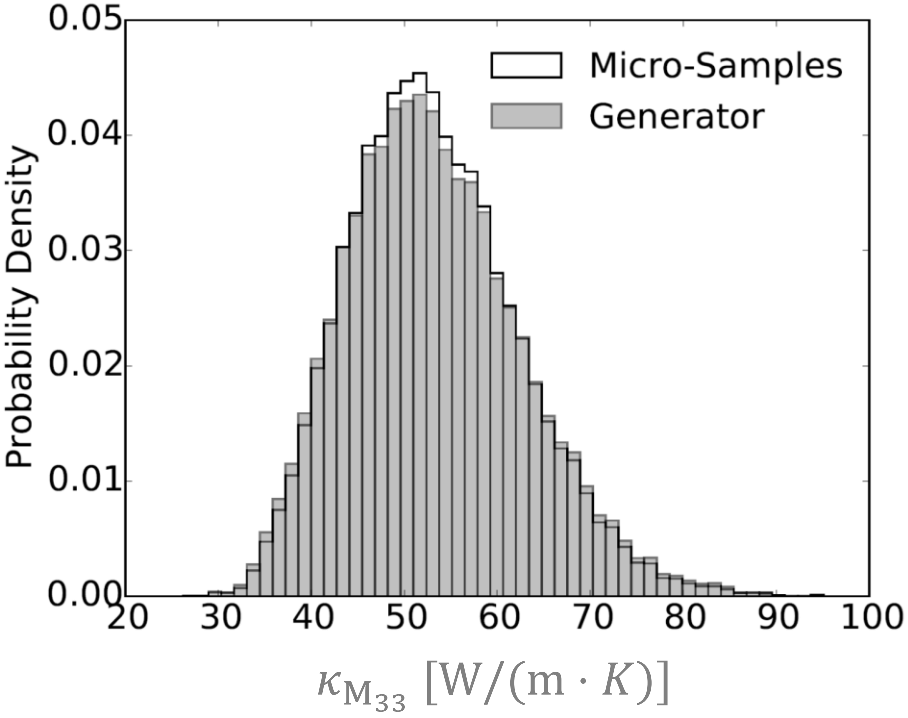
*"*Deodatis, G., Micaletti, R., 2001*

The meso-scale random field

- Polysilicon film deposited at 610 ºC
  - SVE size of 0.5 x 0.5 $\mu\mathrm{m}^2$
  - Comparison between micro-samples and generated field PDFs

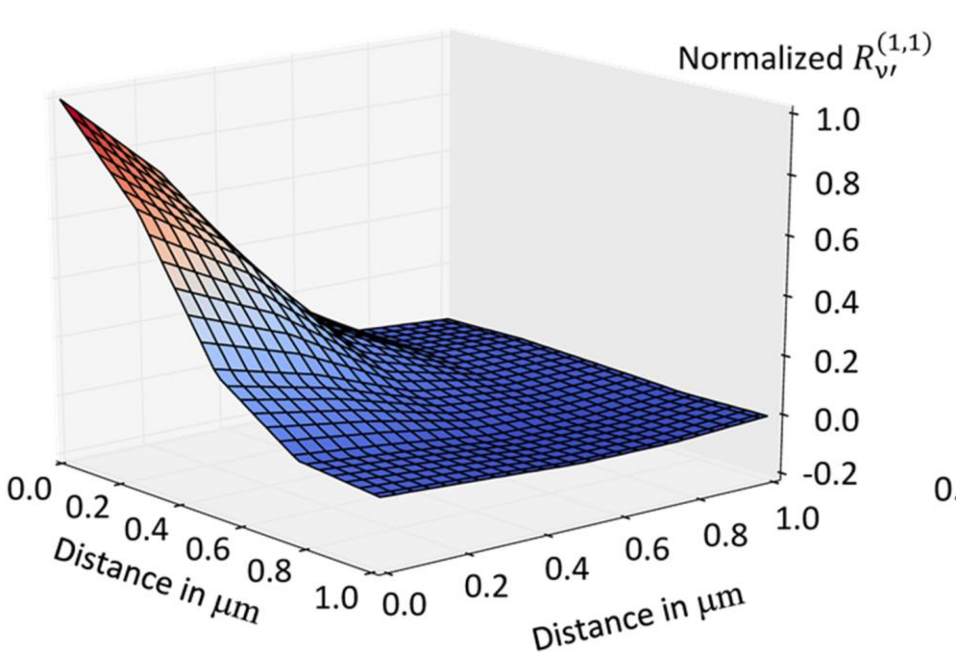




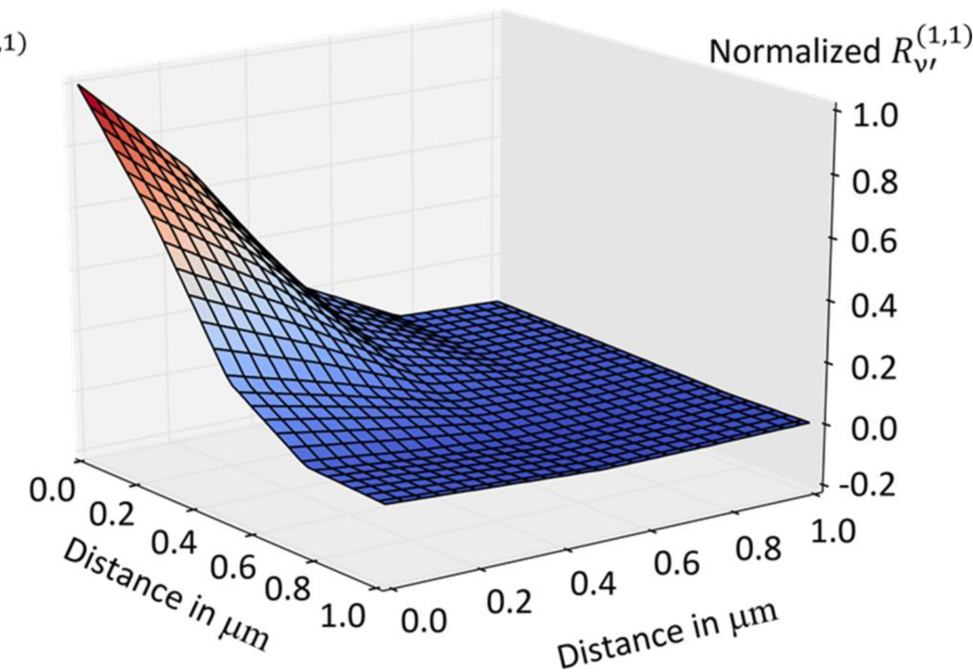


The meso-scale random field

- Polysilicon film deposited at 610 ºC (2)
  - Comparison between micro-samples and generated field cross-correlations

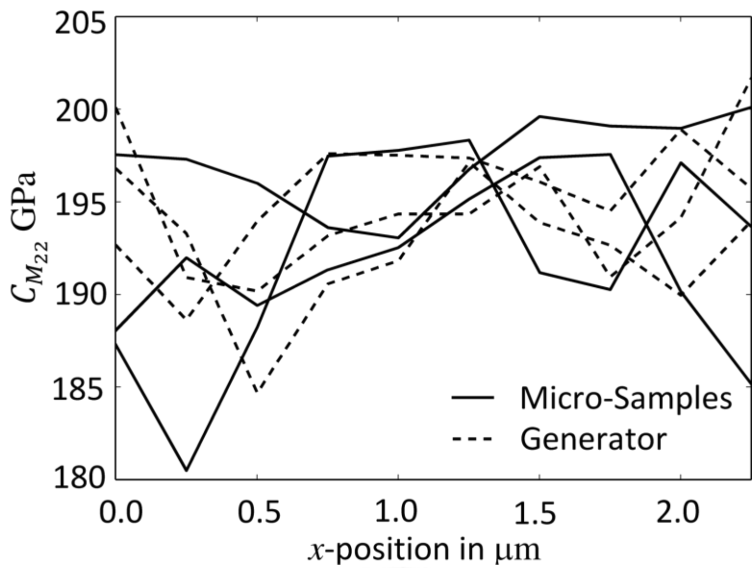


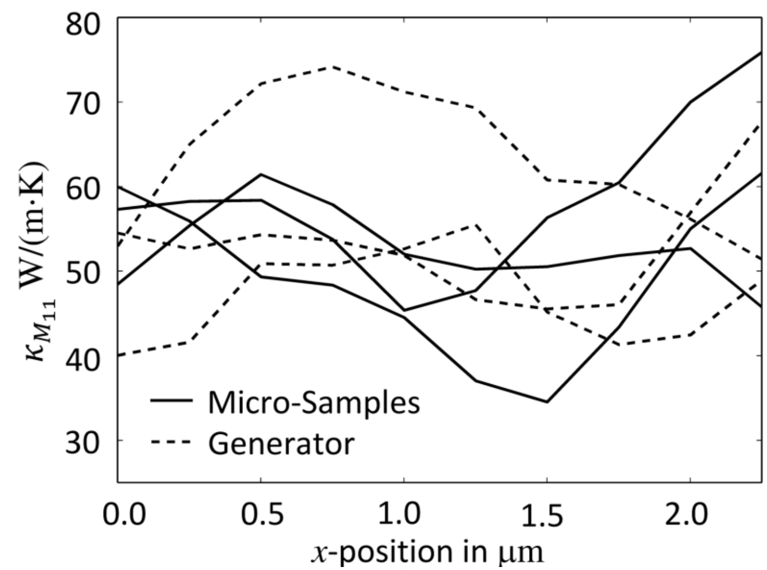
Micro-Samples

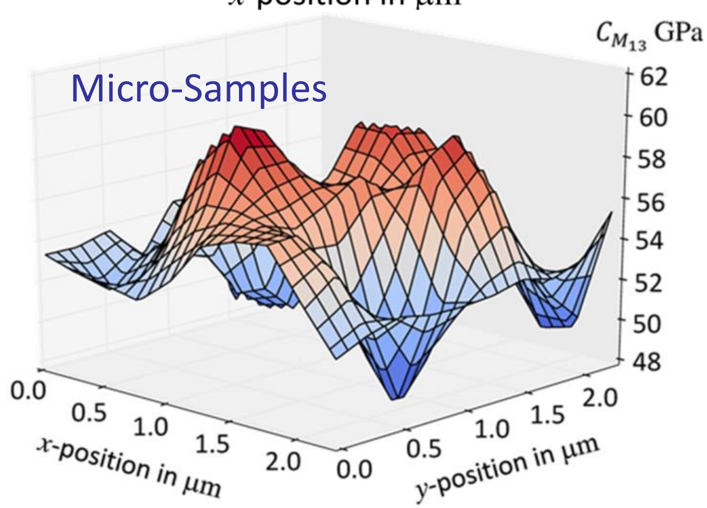


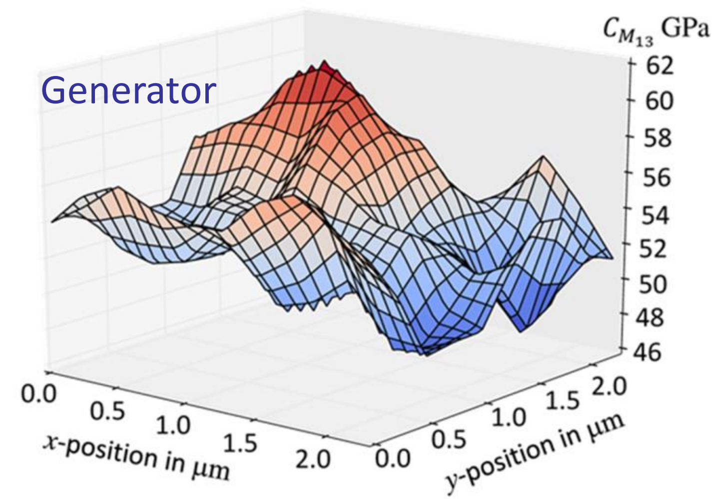
Generator

- Polysilicon film deposited at 610 ºC (3)
  - Comparison between micro-samples and generated random field realizations







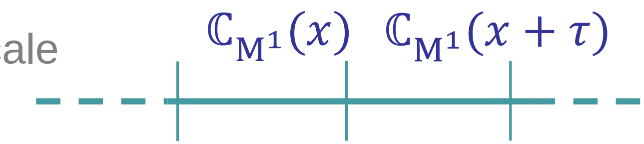


Content

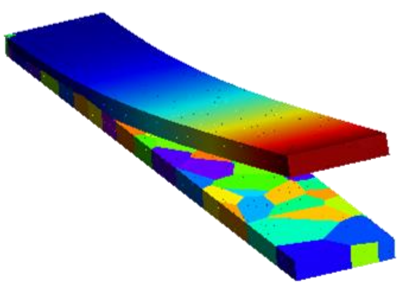
- From the micro-scale to the meso-scale
  - Thermo-mechanical homogenization
  - Definition of Stochastic Volume Elements (SVEs) & Stochastic homogenization
  - Need for a meso-scale random field
- The meso-scale random field
  - Definition of the thermo-mechanical meso-scale random field
  - Stochastic model of the random field: Spectral generator & non-Gaussian mapping
- From the meso-scale to the macro-scale
  - 3-Scale approach verification
  - Application to extract the quality factor
- Accounting for roughness effect
  - From the micro-scale to the meso-scale
  - The meso-scale random field
  - From the meso-scale to the macro-scale

- 3-Scale approach verification with direct Monte-Carlo simulations
  - Use of the meso-scale random field

    → Monte-Carlo simulations at the macro-scale

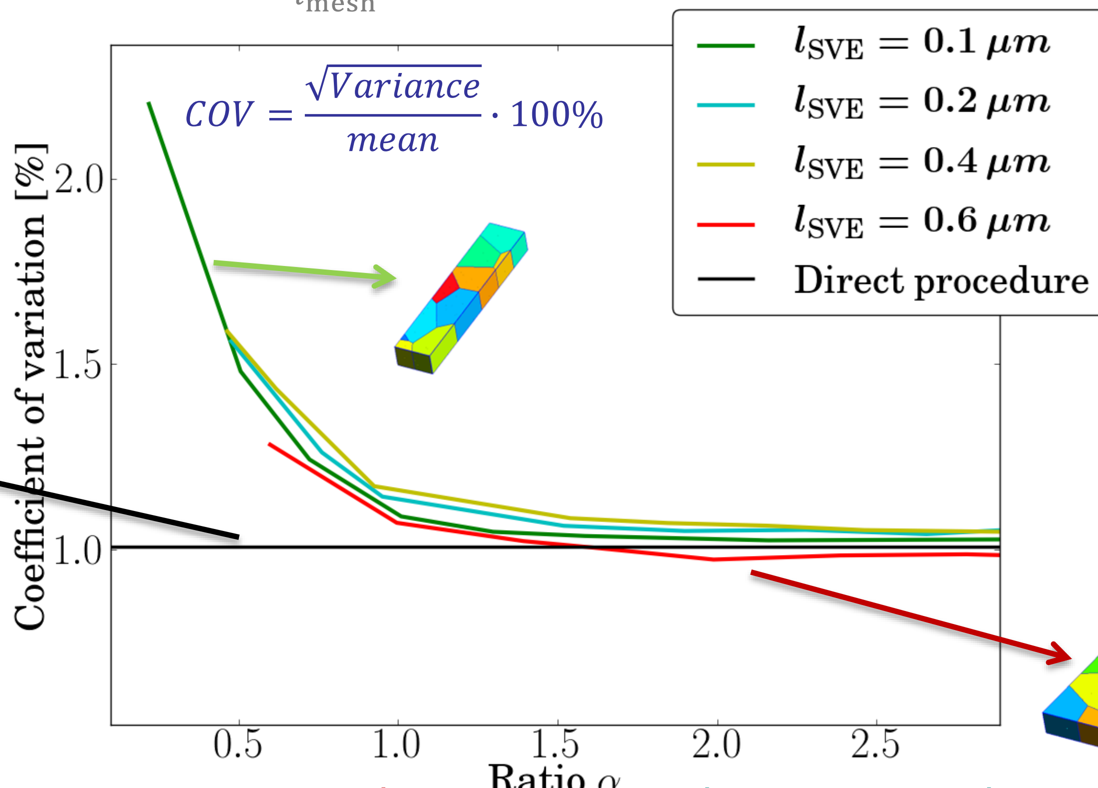


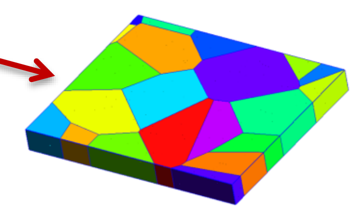
  - Macro-scale beam elements of size l_{mesh}
  - Convergence in terms of $\alpha = \frac{l_{E_x}}{l_{\text{mesh}}}$



First bending mode of

a 3.2 μm-long beam

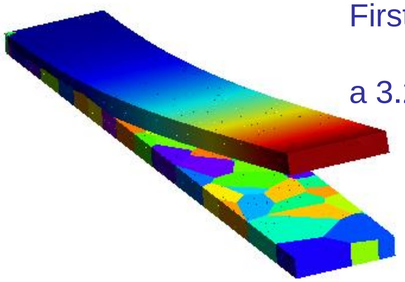




Coarse macro-mesh

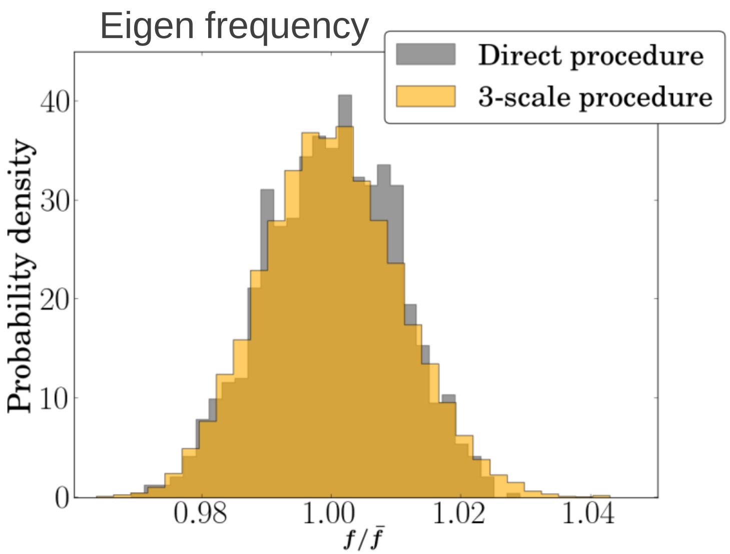
Fine macro-mesh

- 3-Scale approach verification ($\alpha \sim 2$) with direct Monte-Carlo simulations
  - First bending mode

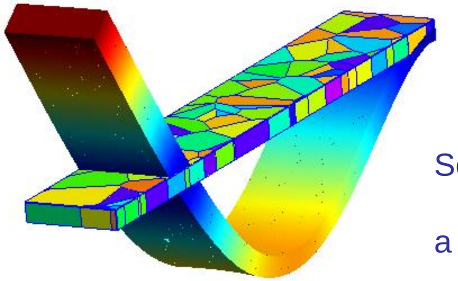


First bending mode of

a 3.2 μm-long beam

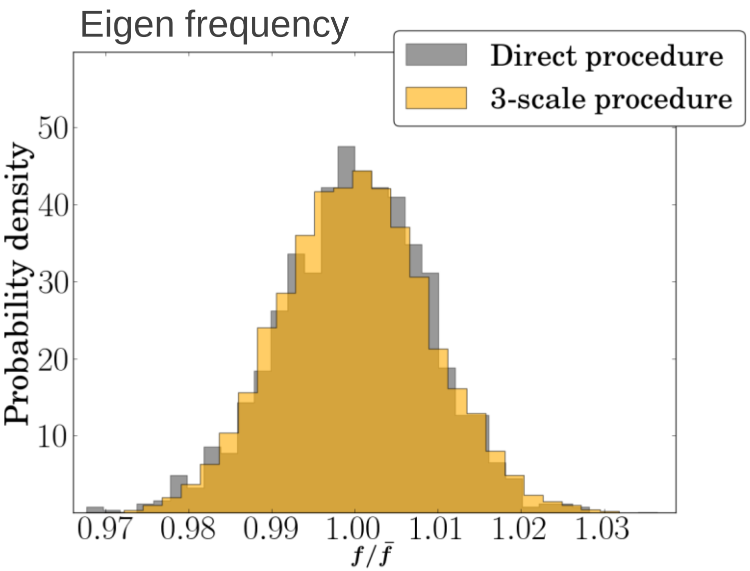


  - Second bending mode

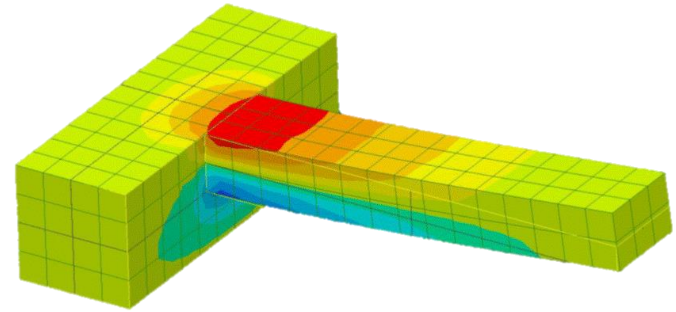


Second bending mode of

a 3.2 μm-long beam



- Quality factor
  - Micro-resonators
    - Temperature changes with compression/traction
    - Energy dissipation



  - Eigen values problem
    - Governing equations

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\mathrm{u}\vartheta}(\boldsymbol{\theta}) & \mathbf{D}_{\vartheta\vartheta} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\mathrm{uu}}(\boldsymbol{\theta}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\theta}) \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\theta}) \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_{\mathrm{u}} \\ \boldsymbol{F}_{\vartheta} \end{bmatrix}$$

    - Free vibrating problem

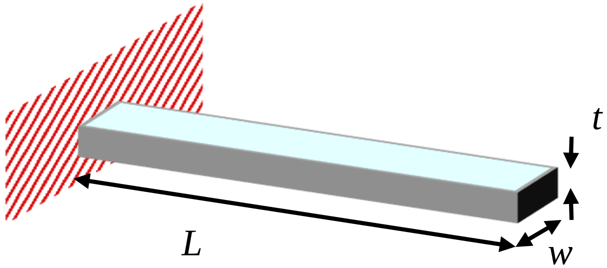
$$\begin{bmatrix} \mathbf{u}(t) \\ \boldsymbol{\vartheta}(t) \end{bmatrix} = \begin{bmatrix} \mathbf{u}_0 \\ \boldsymbol{\vartheta}_0 \end{bmatrix} e^{i\omega t}$$

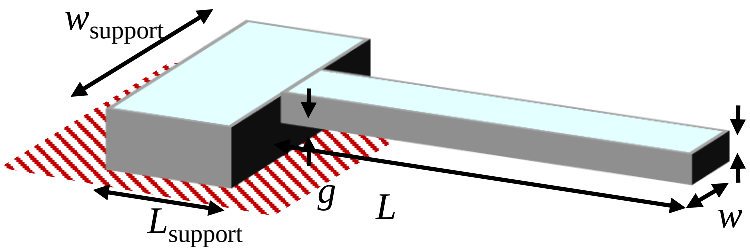
$$\begin{bmatrix} -\mathbf{K}_{\mathrm{uu}}(\boldsymbol{\theta}) & -\mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\theta}) & \mathbf{0} \\ \mathbf{0} & -\mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\theta}) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \\ \dot{\mathbf{u}} \end{bmatrix} = i\omega \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{M} \\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\theta}) & \mathbf{D}_{\vartheta\vartheta} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \\ \dot{\mathbf{u}} \end{bmatrix}$$

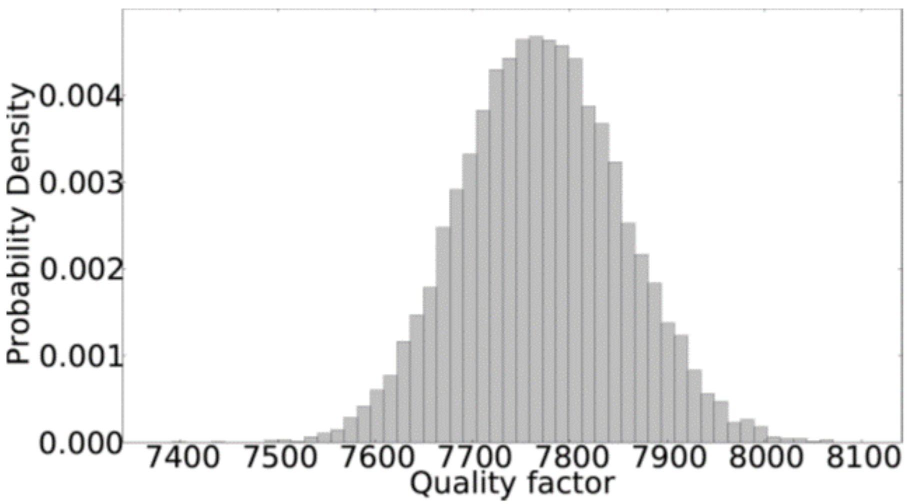
  - Quality factor
    - From the dissipated energy per cycle
    - $Q^{-1} = \dfrac{2|\Im\omega\ |}{\sqrt{(\Im\omega)^2 + (\Re\omega)^2}}$

From the meso-scale to the macro-scale

- Application of the 3-Scale method to extract the quality factor distribution
  - 3D models readily available
  - The effect of the anchor can be studied

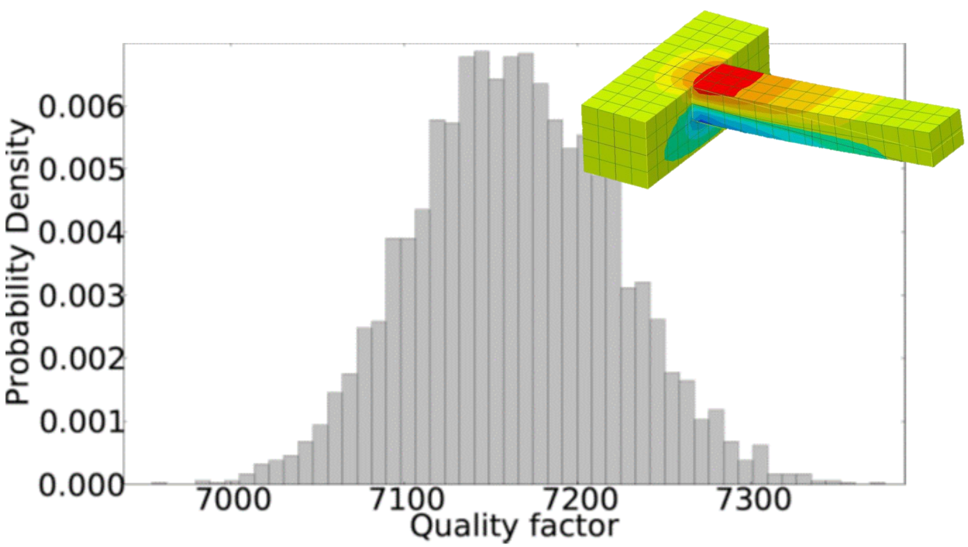






15 x 3 x 2 μm^3-beam,

deposited at 610 ºC



15 x 3 x 2 μm^3-beam & anchor,

deposited at 610 ºC

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- From the micro-scale to the meso-scale
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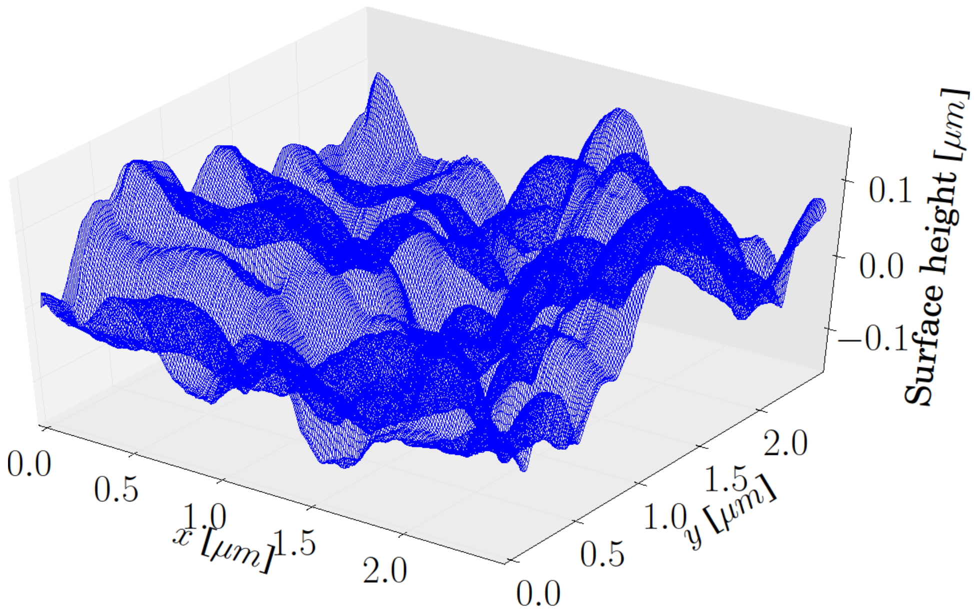
  - The meso-scale random field
  - From the meso-scale to the macro-scale

Accounting for roughness effect

- Surface topology: asperity distribution
  - Upper surface topology by AFM (Atomic Force Microscope) measurements on 2 µm-thick poly-silicon films



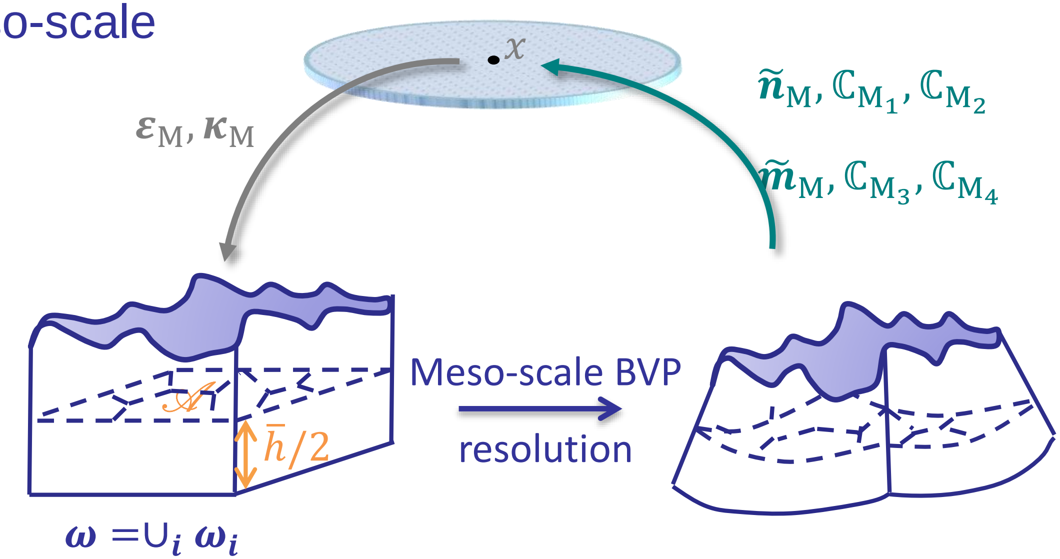
Deposition temperature [°C]	580	610	630	650
Std deviation [nm]	35.6	60.3	90.7	88.3

AFM data provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

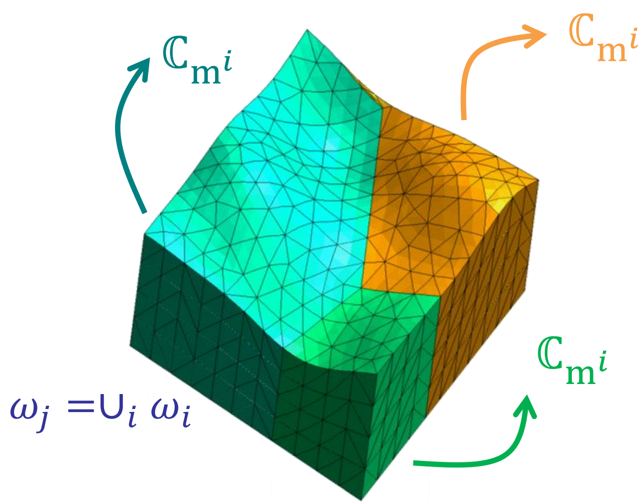
Accounting for roughness effect

- From the micro-scale to the meso-scale
  - Second-order homogenization

$$\begin{cases} \tilde{\boldsymbol{n}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_1} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_2} : \boldsymbol{\kappa}_{\mathrm{M}} \\ \tilde{\boldsymbol{m}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_3} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_4} : \boldsymbol{\kappa}_{\mathrm{M}} \end{cases}$$



  - Stochastic homogenization
    - Several SVE realizations
    - For each SVE $\omega_j = \cup_i \omega_i$
    - The density per unit area is now non-constant



$\mathbb{C}_{\mathrm{m}^i}\ \forall i \longrightarrow \mathbb{C}_{\mathrm{M}_1^j}, \mathbb{C}_{\mathrm{M}_2^j}, \mathbb{C}_{\mathrm{M}_3^j}, \mathbb{C}_{\mathrm{M}_4^j} \longrightarrow \mathrm{U}_{\mathrm{M}^j}$

Computational homogenization

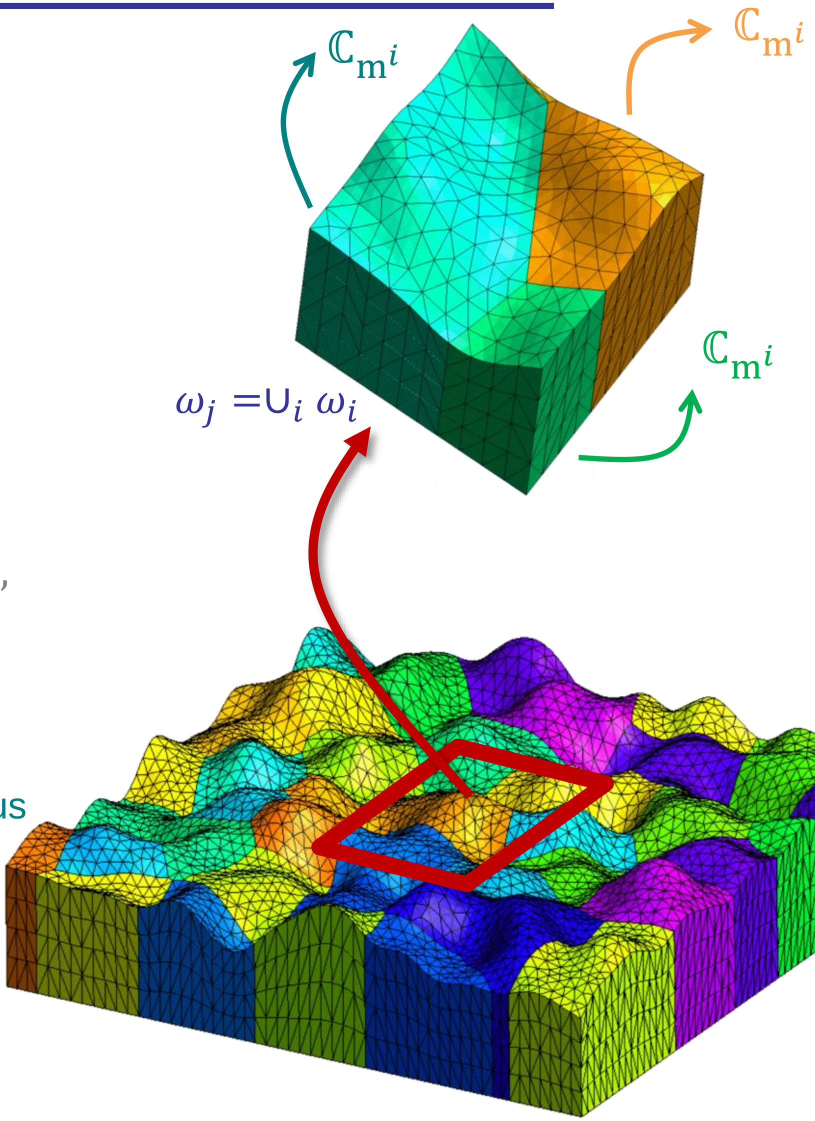
$\bar{\boldsymbol{\rho}}_{\mathrm{M}^j}$

Samples of the meso-scale homogenized elasticity matrix U_{M} & density $\bar{\boldsymbol{\rho}}_{\mathrm{M}}$

Accounting for roughness effect

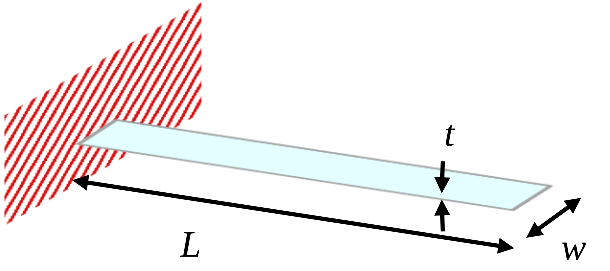
- The meso-scale random field
  - Generate large tessellation realizations
  - For each tessellation realization
    - Extract SVEs centred at $\boldsymbol{x}+\boldsymbol{\tau}$
    - For each SVE evaluate $\mathrm{U}_{\mathrm{M}}(\boldsymbol{x}+\boldsymbol{\tau})$, $\overline{\boldsymbol{\rho}}_{\mathrm{M}}(\boldsymbol{x}+\boldsymbol{\tau})$
  - From the set of realizations $\mathrm{U}_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta})$,$\overline{\boldsymbol{\rho}}_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta})$,
    - Evaluate the bounds $\mathbf{U}_{\mathrm{L}}$ and $\overline{\boldsymbol{\rho}}_{L}$
    - Apply the Cholesky decomposition ⇒ $\boldsymbol{\mathcal{A}}'(\boldsymbol{x},\boldsymbol{\theta})$
    - Fill the 22 entries of the zero-mean homogenous field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x},\boldsymbol{\theta})$
  - Compute the auto-/cross-correlation matrix

$$R_{\boldsymbol{\mathcal{V}}'}^{(rs)}(\boldsymbol{\tau}) = \frac{\mathbb{E}\left[\boldsymbol{\mathcal{V}}'^{(r)}(\boldsymbol{x})\boldsymbol{\mathcal{V}}'^{(s)}(\boldsymbol{x}+\boldsymbol{\tau})\right]}{\sqrt{\mathbb{E}[(\boldsymbol{\mathcal{V}}'^{(r)})^2]\mathbb{E}[(\boldsymbol{\mathcal{V}}'^{(s)})^2]}}$$



Accounting for roughness effect

- From the meso-scale to the macro-scale
  - Cantilever of 8 x 3 x t μm^3 deposited at 610 ºC



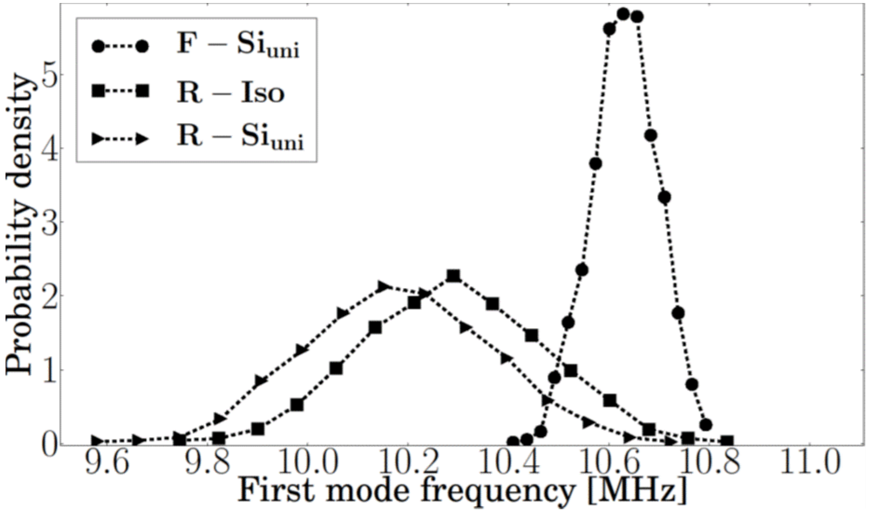
Flat SVEs (no roughness) - F

Rough SVEs (Polysilicon film deposited at 610 ºC) - R

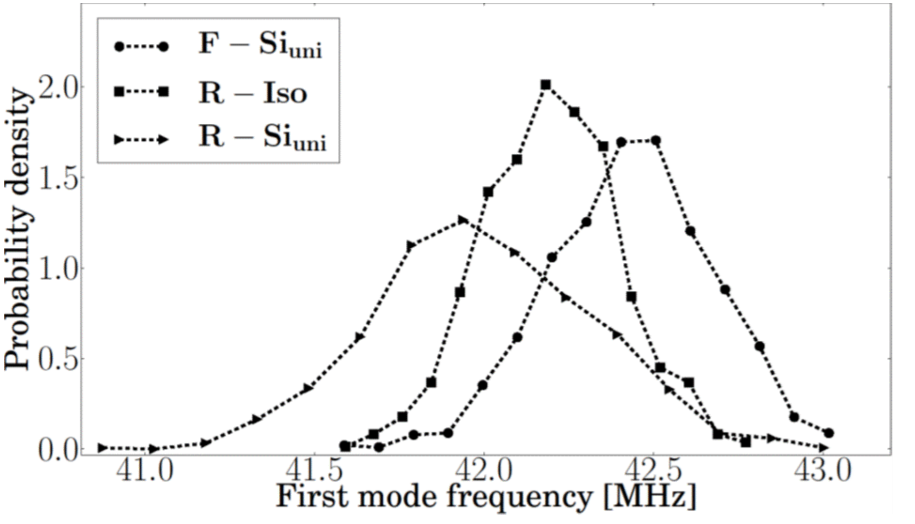
Grain orientation following XRD measurements – Si_{pref}

Grain orientation uniformly distributed – Si_{uni}

Reference isotropic material – Iso



Roughness effect is the most important for 8 x 3 x 0.5 μm^3 cantilevers



Roughness effect is of same importance as orientation for 8 x 3 x 2 μm^3 cantilevers

Conclusions & Perspectives

- Efficient stochastic multi-scale method
  - Micro-structure based on experimental measurements
  - Computational efficiency relies on the meso-scale random field generator
  - Used to study probabilistic behaviors

- Perspectives
  - Other material systems
  - Non-linear behaviors
  - Non-homogenous random fields

Thank you for your attention !

Thermo-mechanical problem

- Governing equations
  - Thermo-mechanics
    - Linear balance $\rho\ddot{\mathbf{u}} - \nabla\cdot\boldsymbol{\sigma} - \rho\boldsymbol{b} = 0$
    - Clausius-Duhem inequality in terms of volume entropy rate $\dot{S} = -\dfrac{\nabla\cdot\boldsymbol{q}}{T}$
    - Helmholtz free energy

$$\begin{cases} \mathcal{F}(\boldsymbol{\varepsilon},T) = \mathcal{F}_0(T) - \boldsymbol{\varepsilon}:\dfrac{\partial^2\psi}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}}:\alpha(T-T_0) + \psi(\boldsymbol{\varepsilon}) \\ \boldsymbol{\sigma} = \left(\dfrac{\partial\mathcal{F}}{\partial\boldsymbol{\varepsilon}}\right)_T \quad , \quad S = \left(\dfrac{\partial\mathcal{F}}{\partial T}\right)_{\boldsymbol{\varepsilon}} \quad \& \quad \left(\dfrac{\partial^2\mathcal{F}_0}{\partial T\partial T}\right) = \rho C_v \end{cases}$$

  - Strong form in terms of the displacements $\boldsymbol{u}$ and temperature change ϑ (linear elasticity)

$$\begin{cases} \rho\ddot{\mathbf{u}} - \nabla\cdot(\mathbb{C}:\dot{\boldsymbol{\varepsilon}} - \mathbb{C}:\boldsymbol{\alpha}\vartheta) - \rho\boldsymbol{b} = 0 \\ \rho C_v\dot{\vartheta} + T_0\boldsymbol{\alpha}:\mathbb{C}:\dot{\boldsymbol{\varepsilon}} - \nabla\cdot(\boldsymbol{\kappa}\nabla\vartheta) = 0 \end{cases}$$

  - Finite element discretization

$$\begin{bmatrix} \mathbf{M}(\rho) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\alpha},\mathbb{C}) & \mathbf{D}_{\vartheta\vartheta}(\rho C_v) \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\mathrm{uu}}(\mathbb{C}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\alpha},\mathbb{C}) \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\kappa}) \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_{\mathrm{u}} \\ \boldsymbol{F}_{\vartheta} \end{bmatrix}$$

The meso-scale random field

- Stochastic model of the meso-scale random field: Spectral generator*
  - Start from the auto-/cross-covariance matrix

$$\tilde{R}^{(rs)}_{\mathcal{V}'}(\boldsymbol{\tau}) = \sigma_{\mathcal{V}'^{(r)}}\sigma_{\mathcal{V}'^{(s)}} R^{(rs)}_{\mathcal{V}'}(\boldsymbol{\tau}) = \mathbb{E}\left[\left(\mathcal{V}'^{(r)}(\boldsymbol{x}) - \mathbb{E}\left(\mathcal{V}'^{(r)}\right)\right)\left(\mathcal{V}'^{(s)}(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}\left(\mathcal{V}'^{(s)}\right)\right)\right]$$

  - Evaluate the spectral density matrix from the periodized zero-padded matrix $\widetilde{\boldsymbol{R}}^{\mathrm{P}}_{\mathcal{V}'}(\boldsymbol{\tau})$

$$\boldsymbol{S}^{(rs)}_{\mathcal{V}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right] = \sum_{n} \widetilde{R}^{\mathrm{P}}_{\mathcal{V}'}{}^{(rs)}\left[\boldsymbol{\tau}^{(\boldsymbol{n})}\right] e^{-2\pi i \boldsymbol{\tau}^{(n)}\cdot\boldsymbol{\omega}^{(\boldsymbol{m})}} \quad \& \quad \boldsymbol{S}_{\mathcal{V}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right] = \boldsymbol{H}_{\mathcal{V}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]\boldsymbol{H}^{*}_{\mathcal{V}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]$$

    - $\boldsymbol{\omega}$ gathers the discrete frequencies
    - $\boldsymbol{\tau}$ gathers the discrete spatial locations
  - Generate a Gaussian random field $\mathcal{V}'(\boldsymbol{x},\boldsymbol{\theta})$

$$\mathcal{V}'^{(r)}(\boldsymbol{x},\boldsymbol{\theta}) = \sqrt{2\Delta\omega}\,\Re\left(\sum_{s}\sum_{\boldsymbol{m}} \boldsymbol{H}^{(\boldsymbol{rs})}_{\mathcal{V}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]\eta^{(s,\boldsymbol{m})}\, e^{2\pi i\left(\boldsymbol{x}\cdot\boldsymbol{\omega}^{(\boldsymbol{m})}+\boldsymbol{\theta}^{(s,\boldsymbol{m})}\right)}\right)$$

    - $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$ are independent random variables
  - Quid if a non-Gaussian distribution is sought?

Shinozuka, M., Deodatis, G., 1988

The meso-scale random field

- Stochastic model of the meso-scale random field: non-Gaussian mapping*
  - Start from micro-sampling of the stochastic homogenization
    - The continuous form of the targeted PSD function

$$\boldsymbol{S}^{\mathrm{T}^{(rs)}}(\boldsymbol{\omega}) = \boldsymbol{\Delta\tau}\boldsymbol{S}^{(rs)}_{\mathcal{V}'}\left[\boldsymbol{\omega}^{(m)}\right] = \boldsymbol{\Delta\tau}\sum_{n}\widetilde{R}^{\mathrm{P}}_{\mathcal{V}'}{}^{(rs)}\left[\boldsymbol{\tau}^{(n)}\right]e^{-2\pi i\boldsymbol{\tau}^{(n)}\cdot\boldsymbol{\omega}^{(m)}}$$

    - The targeted marginal distribution density function $\boldsymbol{F}^{\mathrm{NG}(\boldsymbol{r})}$ of the random variable $\boldsymbol{\mathcal{V}}'^{(\boldsymbol{r})}$
    - A marginal Gaussian distribution $\boldsymbol{F}^{\boldsymbol{G}(\boldsymbol{r})}$ of zero-mean and targeted variance $\boldsymbol{\sigma}_{\boldsymbol{\mathcal{V}}'^{(r)}}$
  - Iterate

Generate Gaussian random vector $\boldsymbol{\mathcal{V}}'^{\mathrm{G}}(\boldsymbol{x})$ from $\boldsymbol{S}^{(rs)}(\boldsymbol{\omega})$

Map $\boldsymbol{\mathcal{V}}'^{\boldsymbol{G}}(\boldsymbol{x})$ to a non-Gaussian field:
$\boldsymbol{\mathcal{V}}'^{\mathrm{NG}^{(r)}}(\boldsymbol{x}) = \boldsymbol{F}^{\mathrm{NG}(\boldsymbol{r})^{-1}}\left(\boldsymbol{F}^{\mathrm{G}(\boldsymbol{r})}\left(\boldsymbol{\mathcal{V}}'^{\mathrm{G}^{(r)}}(\boldsymbol{x})\right)\right)$

Evaluate the PSD $\boldsymbol{S}^{\mathrm{NG}^{(rs)}}(\boldsymbol{\omega})$ of $\boldsymbol{\mathcal{V}}'^{\mathrm{NG}}(\boldsymbol{x})$

$\boldsymbol{S}^{\mathrm{NG}^{(rs)}} \simeq \boldsymbol{S}^{\mathrm{T}^{(rs)}}?$

No

$\boldsymbol{S}^{(rs)}(\boldsymbol{\omega}) \leftarrow \boldsymbol{S}^{(rs)}(\boldsymbol{\omega})\dfrac{\boldsymbol{S}^{\mathrm{T}^{(rr)}}(\boldsymbol{\omega})\boldsymbol{S}^{\mathrm{T}^{(ss)}}(\boldsymbol{\omega})}{\boldsymbol{S}^{\mathrm{NG}^{(rr)}}(\boldsymbol{\omega})\boldsymbol{S}^{\mathrm{NG}^{(ss)}}(\boldsymbol{\omega})}$

*“*Deodatis, G., Micaletti, R., 2001*