A stochastic multiscale method applied to thermo-elasticity analyses of polycrystalline micro-structures

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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
  - As a result, their macroscopic properties can exhibit a scatter
    - Due to the fabrication process (photolithography, wet and dry etching)
    - Due to uncertainties of the material
    - ...

  The objective of this work is to estimate this scatter
The problem

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

\[ \tau \ll T \quad \text{isothermal process} \]
\[ \tau \gg T \quad \text{adiabatic process} \]
\[ \tau \sim T \quad Q \downarrow \]
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

<table>
<thead>
<tr>
<th>Deposition temperature [°C]</th>
<th>580</th>
<th>610</th>
<th>630</th>
<th>650</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Average grain diameter [µm]</strong></td>
<td>0.21</td>
<td>0.45</td>
<td>0.72</td>
<td>0.83</td>
</tr>
</tbody>
</table>

Deposition temperature: 580 °C

Deposition temperature: 650 °C

SEM 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
Motivations

- **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**

  \[ L_{\text{macro}} \gg L_{\text{VE}} \gg L_{\text{micro}} \]

  - **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

\[ L_{\text{macro}} \gg L_{\text{VE}} \sim L_{\text{micro}} \]

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

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

*M Ostoj-Starzewski, X Wang, 1999
P Trovalusci, M Ostoja-Starzewski, M L De Bellis, A Murrari, 2015
X. Yin, W. Chen, A. To, C. McVeigh, 2008
J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem, 2011
...
A 3-scale process

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

![Diagram showing the process]

- Stochastic Homogenization
- Mean value of material property
- Variance of material property
- SFEM
- Probability density
- Quantity of interest

Mean value of material property
Variance of material property
SVE size
Probability density
Quantity of interest
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
Content

• From the micro-scale to the meso-scale
  – Thermo-mechanical homogenization
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• 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
• Definition of Stochastic Volume Elements (SVEs)
  – Poisson Voronoï tessellation realizations
    • SVE realization \( \omega_j \)
  – Each grain \( \omega_i \) is assigned material properties
    • Elasticity tensor \( C_{m_i} \);
    • Heat conductivity tensor \( \kappa_{m_i} \);
    • Thermal expansion tensors \( \alpha_{m_i} \).
    • Defined from silicon crystal properties
  – Each set \( C_{m_i}, \kappa_{m_i}, \alpha_{m_i} \) is assigned a random orientation
    • Following XRD distributions

• Stochastic homogenization
  – Several SVE realizations
  – For each SVE \( \omega_j = \bigcup_i \omega_i \)
    \( C_{m_i}, \kappa_{m_i}, \alpha_{m_i} \quad \forall i \)

*“C. Huet, 1990

**From the micro-scale to the meso-scale**

- Homogenized material tensors not unique as statistical representativeness is lost*
From the micro-scale to the meso-scale

- **Thermo-mechanical homogenization**
  - Down-scaling
    
    \[
    \varepsilon_M = \frac{1}{V(\omega)} \int_{\omega} \varepsilon_m d\omega
    \]

    \[
    \nabla_M \vartheta_M = \frac{1}{V(\omega)} \int_{\omega} \nabla_m \vartheta_m d\omega
    \]

    \[
    \vartheta_M = \frac{1}{V(\omega)} \int_{\omega} \frac{\rho_m C_{vm}}{\rho_M C_{\nu M}} \vartheta_m d\omega
    \]

  - Up-scaling
    
    \[
    \sigma_M = \frac{1}{V(\omega)} \int_{\omega} \sigma_m d\omega
    \]

    \[
    q_M = \frac{1}{V(\omega)} \int_{\omega} q_m d\omega
    \]

    \[
    \rho_M C_{\nu M} = \frac{1}{V(\omega)} \int \rho_m C_{vm} dV
    \]

  - Consistency
    
    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

\[
COV = \frac{\sqrt{\text{Variance}}}{\text{mean}} \cdot 100\%
\]
From the micro-scale to the meso-scale

- 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

\[
COV = \frac{\sqrt{\text{Variance}}}{\text{mean}} \cdot 100\%
\]

First bending mode of a 3.2 µm-long beam
From the micro-scale to the meso-scale

- Use of the meso-scale distribution with macro-scale finite elements
  - Beam macro-scale finite elements
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\[ \text{COV} = \frac{\sqrt{\text{Variance}}}{\text{mean}} \cdot 100\% \]

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

First bending mode of a 3.2 μm-long beam
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

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

- 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 $L_{Ex}$
  - The correlation length $L_{Ex}$ depends on the SVE size

Random field with different SVEs sizes

$l_{SVE} = 0.1 \mu m$

$l_{SVE} = 0.4 \mu m$

- Young's modulus [GPa]
- x position [\mu m]
- $\mathbb{E}[E_x]$ 
- $\mathbb{E}[E_x] \pm \sigma_{E_x}$
- Samples of the random field
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  – From the micro-scale to the meso-scale
  – The meso-scale random field
  – From the meso-scale to the macro-scale
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

Stochastic model of meso-scale elasticity tensors

\[ \mathbb{C}_M(x + \tau, \theta) \]

\[ \mathbb{C}_M(x, \theta) \]

\[ \mathbb{C}_M(x + 2\tau, \theta) \]
The meso-scale random field

- Definition of the thermo-mechanical meso-scale random field
  - Elasticity tensor $C_M(x, \theta)$ (matrix form $C_M$) & thermal conductivity $\kappa_M$ are bounded
    
    - Ensure existence of their inverse
    - Define lower bounds $C_L$ and $\kappa_L$ such that
      
      $\begin{align*}
      &\varepsilon: (C_M - C_L): \varepsilon > 0 \quad \forall \varepsilon \\
      &\nabla \vartheta \cdot (\kappa_M - \kappa_L) \cdot \nabla \vartheta > 0 \quad \forall \nabla \vartheta
      \end{align*}$

  - Use a Cholesky decomposition when semi-positive definite matrices are required
    
    $\begin{align*}
    C_M(x, \theta) &= C_L + (\overline{A} + A'(x, \theta))^T (\overline{A} + A'(x, \theta)) \\
    \kappa_M(x, \theta) &= \kappa_L + (\overline{B} + B'(x, \theta))^T (\overline{B} + B'(x, \theta)) \\
    \alpha_{Mij}(x, \theta) &= \overline{V}^{(t)} + V'(t)(x, \theta)
    \end{align*}$

  - We define the homogenous zero-mean random field $V'(x, \theta)$, with as entries
    
    - Elasticity tensor $A'(x, \theta) \Rightarrow V'(1) ... V'(21)$
    - Heat conductivity tensor $B'(x, \theta) \Rightarrow V'(22) ... V'(27)$
    - Thermal expansion tensors $V'(t) \Rightarrow V'(28) ... V'(33)$
The meso-scale random field

- Characterization of the meso-scale random field
  - Generate large tessellation realizations
  - For each tessellation realization
    - Extract SVEs centered on $x + \tau$
    - For each SVE evaluate $C_M(x + \tau), \kappa_M(x + \tau), \alpha_M(x + \tau)$
  - From the set of realizations $C_M(x, \theta), \kappa_M(x, \theta), \alpha_M(x, \theta)$
    - Evaluate the bounds $C_L$ and $\kappa_L$
    - Apply the Cholesky decomposition $\Rightarrow A'(x, \theta), B'(x, \theta)$
    - Fill the 33 entries of the zero-mean homogenous field $V'(x, \theta)$
  - Compute the auto-/cross-correlation matrix

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

- Generate zero-mean random field $V'(x, \theta)$
  - Spectral generator & non-Gaussian mapping
The meso-scale random field

- Polysilicon film deposited at 610 °C
  - SVE size of 0.5 x 0.5 μm²
  - Comparison between micro-samples and generated field PDFs
The meso-scale random field

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

![Graphs comparing micro-samples and generator results.](image-url)
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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 $l_{\text{mesh}}$
  - Convergence in terms of $\alpha = \frac{l_{E_x}}{l_{\text{mesh}}}$

$$\text{COV} = \sqrt{\text{Variance}} \cdot \frac{\text{mean}}{100\%}$$

![Graph showing coefficient of variation (COV) against ratio $\alpha$.](image)

First bending mode of a 3.2 $\mu$m-long beam
• 3-Scale approach verification ($\alpha \sim 2$) with direct Monte-Carlo simulations
  
  – First bending mode

  ![First bending mode of a 3.2 $\mu$m-long beam](image1)

  
  – Second bending mode

  ![Second bending mode of a 3.2 $\mu$m-long beam](image2)
From the meso-scale to the macro-scale

- **Quality factor**
  - Micro-resonators
    - Temperature changes with compression/traction
    - Energy dissipation
  - Eigen values problem
    - Governing equations
      \[
      \begin{bmatrix}
      M & 0 \\
      0 & 0
      \end{bmatrix}
      \begin{bmatrix}
      \ddot{u} \\
      \ddot{\varphi}
      \end{bmatrix}
      +
      \begin{bmatrix}
      0 & 0 \\
      D_{u\varphi}(\theta) & D_{\varphi\varphi}
      \end{bmatrix}
      \begin{bmatrix}
      \dot{u} \\
      \dot{\varphi}
      \end{bmatrix}
      +
      \begin{bmatrix}
      K_{uu}(\theta) & 0 \\
      0 & K_{\varphi\varphi}(\theta)
      \end{bmatrix}
      \begin{bmatrix}
      u \\
      \varphi
      \end{bmatrix}
      =
      \begin{bmatrix}
      F_u \\
      F_\varphi
      \end{bmatrix}
      \]
    - Free vibrating problem
      \[
      \begin{bmatrix}
      u(t) \\
      \varphi(t)
      \end{bmatrix}
      =
      \begin{bmatrix}
      u_0 \\
      \varphi_0
      \end{bmatrix}
      e^{i\omega t}
      \]
      \[
      \begin{bmatrix}
      -K_{uu}(\theta) & -K_{u\varphi}(\theta) & 0 \\
      0 & -K_{\varphi\varphi}(\theta) & 0 \\
      0 & 0 & 1
      \end{bmatrix}
      \begin{bmatrix}
      u \\
      \varphi
      \end{bmatrix}
      =
      i\omega
      \begin{bmatrix}
      0 & 0 & M \\
      D_{\varphi u}(\theta) & D_{\varphi\varphi} & 0 \\
      0 & 0 & 1
      \end{bmatrix}
      \begin{bmatrix}
      u \\
      \varphi
      \end{bmatrix}
      \]
  - Quality factor
    - From the dissipated energy per cycle
      \[
      Q^{-1} = \frac{2|\Im\omega|}{\sqrt{(\Im\omega)^2 + (\Re\omega)^2}}
      \]
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 μm³-beam, deposited at 610 ºC

15 x 3 x 2 μm³-beam & anchor, deposited at 610 ºC
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  – From the micro-scale to the meso-scale
  – 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

<table>
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<th>610</th>
<th>630</th>
<th>650</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Std deviation [nm]</strong></td>
<td>35.6</td>
<td>60.3</td>
<td>90.7</td>
<td>88.3</td>
</tr>
</tbody>
</table>

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
    \[
    \mathbf{\tilde{\eta}}_M = \mathbf{C}_{M1} : \mathbf{\varepsilon}_M + \mathbf{C}_{M2} : \mathbf{\kappa}_M \\
    \mathbf{\tilde{m}}_M = \mathbf{C}_{M3} : \mathbf{\varepsilon}_M + \mathbf{C}_{M4} : \mathbf{\kappa}_M
    \]
  - Stochastic homogenization
    - Several SVE realizations
    - For each SVE \( \omega_j = \cup_i \omega_i \)
    - The density per unit area is now non-constant

- Computational homogenization
  - Samples of the meso-scale homogenized elasticity matrix \( \mathbf{U}_M \) & density \( \bar{\rho}_M \)

\( \omega = \cup_i \omega_i \)
Accounting for roughness effect

- **The meso-scale random field**
  - Generate large tessellation realizations
  - For each tessellation realization
    - Extract SVEs centred at \( x + \tau \)
    - For each SVE evaluate \( U_M(x + \tau), \bar{\rho}_M(x + \tau) \)
  - From the set of realizations \( U_M(x, \theta), \bar{\rho}_M(x, \theta) \).
    - Evaluate the bounds \( U_L \) and \( \bar{\rho}_L \)
    - Apply the Cholesky decomposition \( \Rightarrow A'(x, \theta) \)
    - Fill the 22 entries of the zero-mean homogenous field \( \mathcal{V}'(x, \theta) \)
  - Compute the auto-/cross-correlation matrix

\[
R_{\mathcal{V}'}^{(rs)}(\tau) = \frac{\mathbb{E} \left[ (\mathcal{V}'^{(r)}(x) - \mathbb{E}(\mathcal{V}'^{(r)})) \left( \mathcal{V}'^{(s)}(x + \tau) - \mathbb{E}(\mathcal{V}'^{(s)}) \right) \right]}{\sqrt{\mathbb{E} \left[ (\mathcal{V}'^{(r)} - \mathbb{E}(\mathcal{V}'^{(r)}))^2 \right]} \mathbb{E} \left[ (\mathcal{V}'^{(s)} - \mathbb{E}(\mathcal{V}'^{(s)}))^2 \right]}
\]
Accounting for roughness effect

- From the meso-scale to the macro-scale
  - Cantilever of $8 \times 3 \times t \mu m^3$ deposited at 610 °C

Flat SVEs (no roughness) - F
Rough SVEs (Polysilicon film deposited at 610 °C) - 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 $8 \times 3 \times 0.5 \mu m^3$ cantilevers
Roughness effect is of same importance as orientation for $8 \times 3 \times 2 \mu m^3$ 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!