Computational & Multiscale Mechanics of Materials





Probabilistic model for MEMS micro-

beam resonance frequency



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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.



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MEMS

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Common denominator: microscopic scale.

MicroElectroMechanical systems

Application in a wide variety of fields

How does it affect the material properties ?

Aeronautics •

Automobile industry

Medecine •

MEMS

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- Telecom •

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The problem

- A macroscopic property of a MEMS can exhibit a scatter
 - Due to the fabrication process
 - Due to uncertainties of the material



The objective of this work is to estimate this scatter

Characteristic of the model:

- Clamped microbeam
- Macroscopic property of interest: first mode eigenfrequency
 - For a MEMS gyroscope for example
- In our model, the uncertainties come from the material:
 - Polysilicon is anisotropic
 - Polysilicon is polycrystalline

Each grain has a random orientation

- Considering each grain to compute the macro quantity is too heavy
 - → 3-scale procedure

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What is the Young's Modulus of Silicon ? ^[1]
 Based on Hall, with *x*, *y*, *z* aligned with [100], [010] and [001], we have:

$oldsymbol{E}_{oldsymbol{\chi}}$ [GPa]	v_{yz}	${\pmb G}_{m yz}$ [GPa]	<i>C</i> ₁₁ [GPa]	<i>C</i> ₁₂ [GPa]	<i>C</i> 44[GPa]
130	0,28	79,6	165,6	63,9	79,5

• Maximum value of *E* in <111> direction: 188 *GPa*



[1] "What is the Young's Modulus of Silicon", M.A. Hopcroft, W.D. Nix, T.W. Kenny, Journal of microelectromechanical systems, april 2010, p.229-238

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A 3-scale procedure

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 ℙ(C) is defined 	 Uncertainty quantification of the macro-scale quantity E.g. the first mode frequency P(f₁) 	
Stochastic Homogenization	Mean value of \overline{E} FE size Variance of \overline{E} FE size	Probability Probability 1 st mode frequency	
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RVE & SVE

- Representative Volume Element (RVE)
 - 1 elasticity tensor : C^{eff}

• Statistical Volume Element (SVE)

- A range of elasticity tensor
 - Depends on boundary conditions
 - Kinematic Uniform BC (KUBC)
 - Periodic BC (PBC)
 - Mixed BC (MBC)
 - Static Uniform BC (SUBC)



Note : A > B iff A - B is positive – definite (Loewner ordering)





Different boundary conditions





SVE of different sizes



When no access to the finite element stiffness matrix K:

 $\boldsymbol{C}_{BC} = \underset{\boldsymbol{C}^{Lower} < \boldsymbol{C} < \boldsymbol{C}^{Upper}}{\arg\min} \| < \boldsymbol{\sigma} >_{BC} - \boldsymbol{C} < \boldsymbol{\epsilon} >_{BC} \|$

- The bounds can be :
 - » Voight & Reuss bounds
 - » KUBC & SUBC
 - In Between (Huet partition theorem [1]) **》**
- E.g., this can happen with concrete experimental samples (see [2])
- When access to the finite element stiffness matrix **K**:
 - The elasticity tensor can be directly computed from the stiffness matrix _
 - This is computational homogenization [5]
 - K^* being a rewritten version of K depending on the boundary condition:

$$\mathbb{C}_{BC} = \frac{1}{V_0} \sum_{i} \sum_{j} \boldsymbol{X}_{(i)} \boldsymbol{K}^*_{(ij)} \boldsymbol{X}_{(j)}$$

- "Application of variational concepts to size effects in elastic heterogenous bodies", Huet C., J.Mech.Phys.Solids, 1990 2
- "A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures", Guilleminot J., Noshadravan A., [3] Soize C., Ghanem R.G., Elsevier, 2011
- "Validation of a probabilistic model for mesoscale elasticity tensor of random polycrystals", Noshadravan A., Ghanem R., Guilleminot J., Atodaria I, [4] International journal for uncertainty quantification, 2011 "Computational homogenization: implementation and extension", Kouznetsova V., Eindhoven University of Technology, 2010
- [5]

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Each are used in [3] and [4]



From micro to meso: results



From micro to meso: results



[3] "A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures", Guilleminot J., Noshadravan A., Soize

C., Ghanem R.G., Elsevier, 2011

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[4] "Validation of a probabilistic model for mesoscale elasticity tensor of random polycrystals", Noshadravan A., Ghanem R., Guilleminot J., Atodaria I, International journal for uncertainty quantification, 2011

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The problem

- If a Monte-Carlo procedure is applied with FEM over a microbeam:
 - No distribution and no generator:
 - For each macro realization
 - At each Gauss points:
 - » a SVE should be computed
 - With distribution and generator:
 - Define a distribution encompassing
 the microstructure statistical behaviour
 - At each Gauss point:
 - Use the generator







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The problem

> 1D case of E_x : Beta-based distribution of 4 parameters

$$P(E_x) = \frac{1}{\beta(\alpha,\beta)} \left[\frac{E_x - E_x^l}{E_x^u - E_x^l} \right]^{\alpha-1} \left[\frac{E_x^u - E_x}{E_x^u - E_x^l} \right]^{\beta-1}$$





Maximize the information entropy •

 $\max_{\mathbb{C}} - \int_{M_{\pi}^{+}(\mathbb{R})} p([\mathbb{C}]) \ln(p([\mathbb{C}])) d\mathbb{C}$

- Under constraints encompassing the available information
 - Samples of C
 - Bounds \mathbb{C}_{i} and \mathbb{C}_{l}
- No change of variable
 - Matrix-variate Kummer-beta distribution [6]
- Using the N space [3,4] \rightarrow N

$$V = \frac{1}{C - C_l} - \frac{1}{C_u - C_l}$$

- Non-linear change of variable
- Matrix-variate Gamma distribution [7]
- Using the N' space \rightarrow N' = C C₁
 - Linear change of variable
 - Matrix-variate Gamma distribution
 - Loose the bound information

[6] "A bounded random matrix approach for stochastic upscaling", S. Das and R. Ghanem, Society for industrial and appl. Math., 2009, [7] "Random matrix theory for modeling uncertainties in computational mechanics", Soize C., Comp. meth. In Appl. Mech. And Engrg., 2004

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- From samples of grain orientations, elasticity tensors can be generated at mesoscale.
- How can we propagate the uncertainties up to the macroscopic scale?
 - Relevant SVE size
 - Correlation
 - ...





- Upgrades can take various forms:
 - 3D meso to macro part
 - Perturbation or Spectral Finite Element
 - Periodic boundary condition for the microstructure

- ...

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Thank you for your attention !

