Propagation of uncertainties using probabilistic multi-scale models

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Abstract

When applying a multiscale approach, the material behavior at the macro-scale can be obtained from an homogenization scheme. To this end, at each integration-point of the macro-structure, the macro-stress tensor is related to the macro-strain tensor through the resolution of a micro-scale boundary value problem. At the micro-level, the macro-point is viewed as the center of a Representative Volume Element (RVE). However, to be representative, the micro-volume-element should have a size much bigger than the micro-structure size.

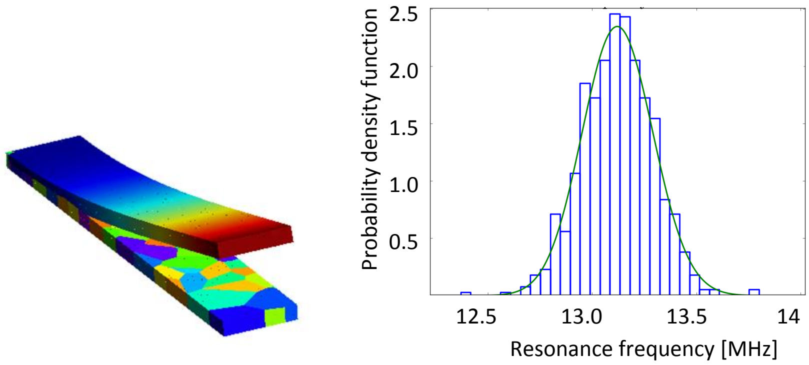
When considering structures of reduced sizes, such as micro-electro-mechanical systems (MEMS), as the size of the devices is only one or two orders of magnitude higher than the size of their micro-structure, *i.e.* their grain size, the structural properties exhibit a scatter at the macro-scale. The representativity of the micro-scale volume element is lost and Statistical Volume Elements (SVE) should be considered in order to account for the micro-structural uncertainties. These uncertainties should then be propagated to the macro-scale in order to predict the device properties in a probabilistic way. In this work we propose a non-deterministic multi-scale approach [1] for poly-silicon MEMS resonators.

A set of SVEs is first generated under the form of Voronoï tessellations with a random orientation assigned for each silicon grain of each SVE. The resolution of each micro-scale boundary problem is performed by recourse to the computational homogenization framework, *e.g.* [2], leading to meso-scale material properties under the form of a linear material tensor for each SVE. Applying a Monte-Carlo procedure allows a distribution of this material tensor to be determined at the meso-scale. The correlation between the meso-scale material tensors of two SVEs separated by a given distance can also be evaluated.

A generator of the meso-scale material tensor is then implemented using the spectral method [3]. The generator [1] accounts for a lower bound [4] of the meso-scale material tensor in order to ensure the existence of the second-order moment of the Frobenius norm of the tensor inverse [5].

A macro-scale finite element model of the beam resonator can now be achieved using regular finite-element, i.e. not conforming with the grains, and the material tensor at each Gauss point is obtained using the meso-scale generator, which accounts for the spatial correlation. A Monte-Carlo method is then used at the macro-scale to predict the probabilistic behavior of the MEMS resonator.

As an example the beam resonator illustrated in Fig. 1(a) is made of poly-silicon, and each grain has a random orientation. Solving the problem with a full direct numerical simulation combined to a Monte-Carlo method allows the probability density function to be computed as illustrated in Fig.



(a) FEM (b) Probability distribution

Figure 1: Non deterministic prediction of the first resonance frequency of a beam resonator (a) Finite element model (FEM) of the beam resonator. (b) Probability density function obtained using a Monte-Carlo method with a random grain distribution.

1(b). However this methodology is computationally expensive due to the number of degrees of freedom required to study one sample. The proposed non-deterministic multi-scale strategy allows reducing this computational cost as the Monte-Carlo processes are applied on much smaller finite-element models.

The method can also be applied in the context of fracture of thin poly-silicon film [6]. In this case, a set of meso-scopic cohesive laws can be obtained at the meso-scale from the resolution of different SVEs. The meso-scopic cohesive laws are obtained for each RVE from the finite element resolution of the Voronoï tessellations using the method proposed in [7]. The resulting statistical values for the critical energy release rate and for the critical strength can then be used for macro-scale simulations.

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References

[1] Lucas, V., Wu, L., Paquay, S., Golinval, J.-C., Noels L. A stochastic computational multiscale approach; application to MEMS resonators. In preparation.

[2] Kouznetsova, V., Brekelmans W. A. M., Baaijens, F. P. T. An approach to micro-macro modeling of heterogeneous materials. *Comput. Mech.*, 27: 37-48, 2001.

[3] Shinozuka, M., Deodatis, G. Simulation of stochastic processes by spectral representation. *Appl. Mech. Rev.*, 1991: 44(4): 191-204, 1991.

[4] Das S., Ghanem, R. A Bounded Random Matrix Approach for Stochastic Upscaling. *Multiscale Modeling & Simulation*, 8(1):296-325, 2009.

[5] Soize, C. Nonlinear dynamical systems with nonparametric model of random uncertainties. *Uncertainties in Engng Mech.*, 1:1-38, 2001.

[6] Mulay, S., Becker, G., Vayrette, R., Raskin, J.-P., Pardoen,T., Galceran, M., Godet, S., Noels, L. Multiscale modelling framework for the fracture of thin brittle polycrystalline films - Application to polysilicon. *Computat. Mech.*, In press.

[7] Verhoosel, C.V., Remmers, J.J.C., Gutiérrez, M.A., de Borst, R. Computational homogenization for adhesive and cohesive failure in quasi-brittle solids. *Inter. J. for Num. Meth. in Engng.*, 83(8-9): 1155-1179, 2010.