Perturbation Stochastic Finite Element Analysis of Thermoelastic Quality Factor of Micro-Resonators

S. Lepage and J.C. Golinval

University of Liege, Aerospace and Mechanical Engineering Department, LTAS-VIS

ABSTRACT

In the design of micro-electromechanical systems (MEMS) such as micro-resonators, one of the major dissipation phenomena to be considered is thermoelastic damping. The performance of such MEMS is directly related to their thermoelastic quality factor which has to be predicted accurately. Moreover, the performance of MEMS depends on manufacturing processes which may cause substantial uncertainty in the geometry and in the material properties of the device. The aim of this paper is to provide a framework to account for uncertainties in the finite element analysis. Particularly, the influence of uncertainties on the performance of a micro-beam is studied using the perturbation stochastic finite element method. The developed method is applied on the analysis of the thermoelastic quality factor of a micro-beam whose elastic modulus is considered as random.

Keywords: stochastic finite element method, thermoelastic damping, micro-resonator, uncertainty modeling.

1 INTRODUCTION

Micro-electromechanical systems (MEMS) are subject to inevitable and inherent uncertainty in dimensional and material parameters, that leads to variability in their performance and reliability. Manufacturing processes due to the small dimensions and high feature complexity leave substantial variability in the shape and geometry of the device while material properties of a component are inherently subject to scattering. The effects of these variations have to be considered and a modeling methodology is needed in order to ensure required MEMS performance under uncertainties.

In the literature, different works are carried out to quantify the effect of the uncertainties on electrostatically actuated MEMS [1]–[4]. These studies consider material and geometric parameters as random variables and use costly Monte-Carlo methods as well as first and second order reliability methods. Another approach to avoid the detrimental effect of these uncertainties is to design MEMS whose performances are not sensitive to the uncertain design parameters [5]–[7], but this is not always possible. In this paper, the Perturbation Stochastic Finite Element Method (PSFEM) is used to quantify the influence of uncertain geometric and material property variations on the thermoelastic quality factor of micro-resonators.

The paper is organized as follows. Firstly, the procedure to quantify the thermoelastic quality factor is exposed. An efficient thermoelastic finite element formulation is the key point in order to investigate the influence of uncertainties on the behavior of micro-systems. Then, the perturbation stochastic finite element method is extended to the study of the thermoelastic quality factor. Finally, the results of PSFEM simulations are presented and discussed.

2 THERMOELASTIC FINITE ELEMENT FORMULATION

Thermoelastic damping represents the loss in energy from an entropy rise caused by the coupling between heat transfer and strain rate. Analytical models exist for simple configurations such as beams [8], [9]. However, a numerical approach is required in order to take into account the spatial variation of the material properties. A thermoelastic finite element formulation is derived in [10] and shows efficiency in order to estimate the thermoelastic quality factor [11].

In order to determine the thermoelastic quality factor, the thermoelastic frequencies λ have to be computed. The eigenvalue problem corresponding to the thermoelastic problem is

$$\begin{pmatrix} -\mathbf{K}_{uu} & -\mathbf{K}_{u\theta} & 0 \\ 0 & -\mathbf{K}_{\theta\theta} & 0 \\ 0 & 0 & \mathbf{M}_{uu} \end{pmatrix} \begin{pmatrix} \mathbf{x}_u \\ \mathbf{x}_\theta \\ \dot{\mathbf{x}}_u \end{pmatrix} = \lambda \begin{pmatrix} 0 & 0 & \mathbf{M}_{uu} \\ \mathbf{C}_{\theta u} & \mathbf{C}_{\theta\theta} & 0 \\ \mathbf{M}_{uu} & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{x}_u \\ \mathbf{x}_\theta \\ \dot{\mathbf{x}}_u \end{pmatrix}, \qquad (1)$$

where subscripts u and θ refer respectively to the mechanical and thermal degrees of freedom. $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$ are respectively mass, damping and stiffness matrices.

If the number of mechanical and thermal degrees of freedom is denoted by n_u and n_θ, respectively, the eigenvalue problem (1) has $2n_u$ conjugate complex eigenvalues and n_θ real eigenvalues. The $2n_u$ eigenvalues correspond to the mechanical frequencies and the n_θ ones to the thermal frequencies. Solving the thermoelastic eigenvalue problem with a non-symmetric block Lanczos algorithm allows the calculation of the complex eigenvalues of the thermoelastic structure and hence, the determination of the quality factor of the corresponding mode. The quality factor of the nth mode is given by

$$Q = \frac{1}{2}\left|\frac{\Im(\lambda)}{\Re(\lambda)}\right|. \tag{2}$$

3 PERTURBATION STOCHASTIC FINITE ELEMENT METHOD

Stochastic Finite Element Method (SFEM) can be applied to the thermoelastic problem. The present work focuses on second moment approaches, in which the first two statistical moments, i.e. the mean and the variance, are estimated. The perturbation SFEM is used in order to determine the mean and the variance of the thermoelastic quality factor of MEMS. The perturbation SFEM [12] consists in a deterministic analysis complemented by a sensitivity analysis with respect to the random parameters. This enables the development of a Taylor series expansion of the response, from which the mean and variance of the response can be derived knowing the mean and variance of the random parameters.

The perturbation method considers that the random design variables b_i are perturbed from their expectation $\bar{b_i}$, so that the random variables b_i are written as the sum of a deterministic value $\bar{b_i}$ and a zero mean random variable Δb_i.

The second order Taylor expansion about the nominal value $\bar{\mathbf{b}}$ with respect to the random variables b_i is given by

$$Q(\bar{\mathbf{b}}) \approx \bar{Q} + \sum_{i=1}^{n} Q_{,i}\Delta b_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{,ij}\Delta b_i \Delta b_j, \tag{3}$$

where the subscripts $,i$ and $,ij$ respectively denote the first and second order partial derivative with respect to b_i and b_j computed at the nominal value $\bar{\mathbf{b}}$.

Since the random variables Δb_i are zero-mean random variables of known covariance, the expectation of the quality factor is

$$\begin{aligned} E\left[Q(\bar{\mathbf{b}})\right] &\approx \bar{Q} + \sum_{i=1}^{n} Q_{,i} E\left[\Delta b_i\right] \\ &\quad + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{,ij} E\left[\Delta b_i \Delta b_j\right] \qquad (4) \\ &= \bar{Q} + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} Q_{,ij} Cov(b_i, b_j), \qquad (5) \end{aligned}$$

while the variance of the quality factor has the following expression:

$$\begin{aligned} Var\left(Q(\bar{\mathbf{b}})\right) &= E\left[\left(Q(\bar{\mathbf{b}}) - E\left[Q(\bar{\mathbf{b}})\right]\right)^2\right] \qquad (6) \\ &\approx \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{,i} Q_{,j} E\left[\Delta b_i \Delta b_j\right] \qquad (7) \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} Q_{,i} Q_{,j} Cov(b_i, b_j). \qquad (8) \end{aligned}$$

The mean is second-order accurate, while the variance is first-order accurate since the second-order terms vanish. The first and second order derivatives of the quality factor are expressed in terms of the first and second order derivatives of the eigenvalue. Due to the nature of the thermoelastic eigenproblem, this study involves the calculation of eigenvalue sensitivities of a non-symmetric damped system [13].

4 APPLICATIONS

In numerous micro-resonators, the vibrating part consists in a clamped-clamped silicon beam. In this section, the test case beam has the following dimensions: a length L of 90 μm, a height h of 4.5 μm and a width w of 4.5 μm (Figure 1). The thermal and mechanical properties of silicon at $T_o = 298\ K$ are: $\rho = 2300\ kg/m^3$, $\nu = 0.2$, $c_v = 711\ J/kgK$, $\alpha = 2.510^{-6}\ K^{-1}$ and $k = 170\ Wm^{-1}K^{-1}$. The thermoelastic quality factor is determined for the first bending mode in plane OYZ.

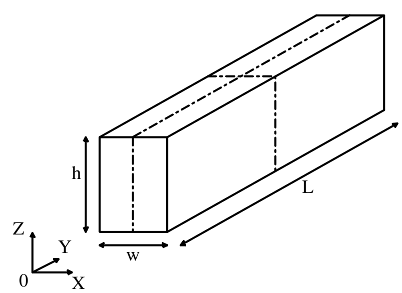

Figure 1: Beam geometry.

Young's modulus is considered as a Gaussian random variable. Its mean is equal to 158 GPa and its coefficient of variation, i.e. the ratio between the standard deviation and the mean, is set to 6 %, which is a typical value encountered in polysilicon. Direct Monte-Carlo simulations are carried out in order to get a reference solution. 2000 samples are generated.

Table 1 lists the means and standard deviations of the quality factor obtained by different methods. Monte-Carlo results, denoted MC, are considered as reference solutions. First and second order perturbation stochastic finite element methods, denoted PSFEM 1st and PS-

NSTI-Nanotech 2007, www.nsti.org, ISBN 1420061844 Vol. 3, 2007

FEM 2nd, are applied to study the thermoelastic quality factor of the test case. Since the determination of the second order derivative of the eigenvalue can be too computationally demanding, a second order PSFEM in terms of the quality factor but only taking into account the first order derivative of the eigenvalue, denoted PSFEM p2nd, is also investigated. The CPU times for each method are normalized with respect to the CPU time required for one deterministic finite element resolution and are presented in Table 1. MC simulations are a lot more CPU time costly than PSFEM and as the order of PSFEM increases, the CPU time increases. Since the approximation of the standard deviation of the quality factor is first order accurate (Equation (7)), the standard deviation has the same value whatever the order of the PSFEM and the relative error with respect to MC standard deviation is less than 1 %. The first order PSFEM gives a mean equal to the deterministic quality factor, i.e. 12967, while MC simulations yield a higher mean. This is due to the fact that the quality factor is a non-linear function of Young's modulus as shown in Figure 2(b). Moreover, due to this non-linear variation, the probability density function of the quality factor is not strictly Gaussian as shown in Figure 2(a). In this figure, the bars represent the distribution of the output samples obtained by MC simulations and the solid line plots the Gaussian distribution with a mean and a standard deviation equal to the values of the MC samples. The second order PSFEM approximation of the mean is really good (0.02 % relative error) and the pseudo second order PSFEM approximation has also a good accuracy (0.026 % relative error) at a less computational effort.

Table 1 also compares the means and standard deviations of the quality factor corresponding to three different coefficients of variation of Young's modulus, i.e. 6 %, 10 % and 20 %. As the coefficient of variation of Young's modulus increases, the approximations of the mean and standard deviation of the quality factor by PSFEM become less accurate. The second order PSFEM is more accurate than the pseudo-second order PSFEM at the price of a considerably larger computational effort. Figures 2(a,c,d) show that as the coefficient of variation of Young's modulus increases, the probability density function drifts away from the Gaussian distribution and PSFEM approximations get worse. Note that as the coefficient of variation increases, the required number of samples in MC simulations increases leading to a larger CPU time($n_{samples} = 5000$ for $CoV = 10\%$ and $n_{samples} = 10000$ for $CoV = 20\%$).

These analyses show that PSFEM is adequate in order to determine the mean and standard deviation of the quality factor when Young's modulus variation is small (i.e. in this application, a coefficient of variation lower than 10 %). The second order and the pseudo-second order perturbation stochastic finite element methods provide more information than the first order one. Indeed, the first order method does not take into account the variation of the mean due to the non-linear characteristic of the response with respect to the random variable. Moreover, the increase in accuracy from PSFEM p2nd to PSFEM 2nd is not sufficient to justify the increase in computational effort.

5 CONCLUSION

The Perturbation Stochastic Finite Element Method has been extended to the analysis of a strongly coupled multiphysic phenomenon: thermoelastic damping. The methodology has been validated and it efficiency has been proved on 1-D cases. Therefore, using PSFEM, a numerical method is available to quantify the influence of uncertain property variations on the thermoelastic quality factor of micro-resonators, making available a new efficient numerical tool to MEMS designers.

REFERENCES

[1] M. Allen, M. Raulli, K. Maute, and D. Frangopol. *Computers and Structures*, 82:1007–1020, 2004.

[2] J.S. Kong, D.M. Frangopol, M. Raulli, K. Maute, R.A. Saravanan, L.-A. Liew, and R. Raj. *Sensors and Actuators A*, 116:336–344, 2004.

[3] K. Maute and D.M. Frangopol. *Computers and Structures*, 81:813–824, 2003.

[4] S. Reh, P. Lethbridge, and D. Ostergaard. *Technical proceedings of the 2000 International Conference on Modeling and Simulation of Microsystems*, pages 708–711, 2000.

[5] R. Liu, B. Paden, and K. Turner. *Journal of Microelectromechanical Systems*, 11(5):505–511, 2002.

[6] A. Mawardi and R. Pitchumani. *Journal of Microelectromechanical Systems*, 14(1), 2005.

[7] A. Mawardi and R. Pitchumani. *Journal of Micromechanics and Microengineering*, 15:2353–2365, 2005.

[8] R. Lifshitz and M.L. Roukes. *Physical Review B*, 61(8):5600–5609, February 2000.

[9] C. Zener. *Physical Review*, 52:230–235, August 1937.

[10] S. Lepage and J.-C. Golinval. In *Acomen 2005, Third International Conference on Advanced Computational Methods in Engineering*, Ghent, Belgium, 30 May-2 June 2005.

[11] S. Lepage, O. Le Traon, I. Klapka, S. Masson, and J.-C. Golinval. In *Caneus 2006*, Toulouse, France, August 27- September 01 2006.

[12] M. Kleiber and T.D. Hien. John Wiley and sons, 1992.

[13] K.M. Choi, H.K. Jo, W.H. Kim, and I.W. Lee. *Journal of Sound and Vibration*, 274:997–1011, 2004.

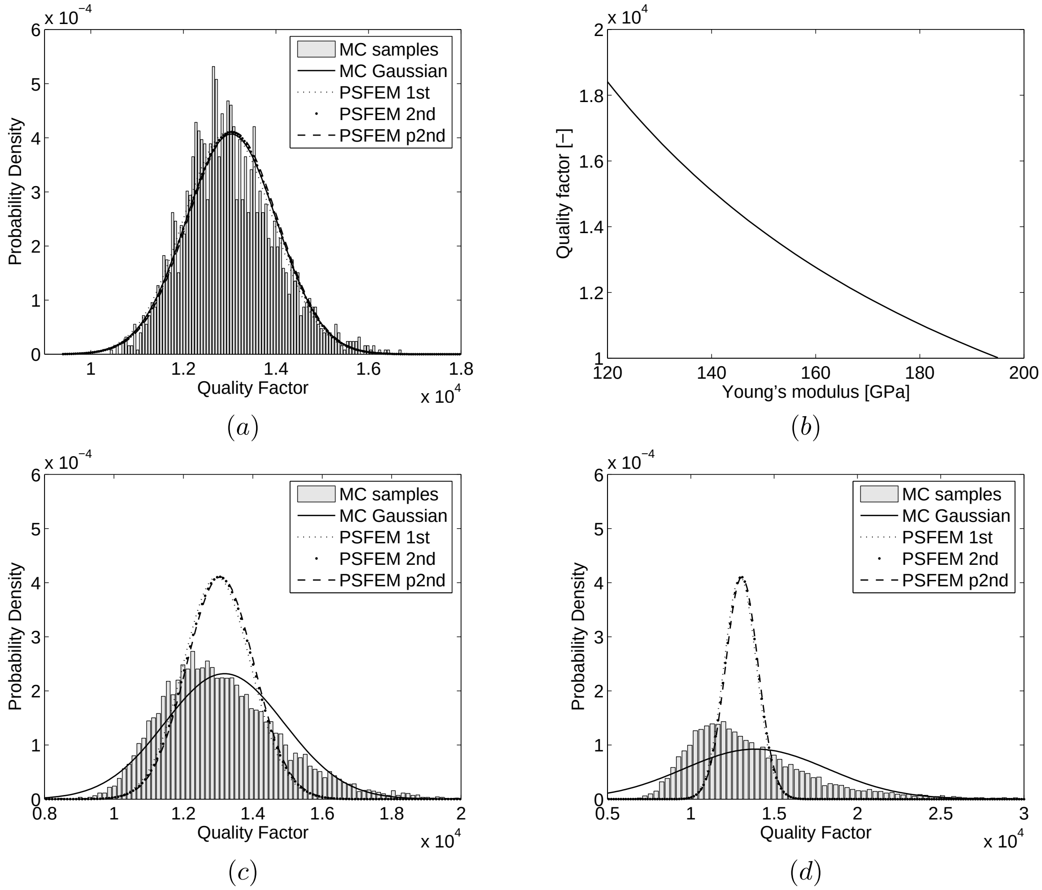

Figure 2: Probability density function of the quality factor (CoV(E)=0.06 (a), CoV(E)=10 % (c) and CoV(E)=20 % (d)), (b) Variation of the quality factor with respect to Young's modulus.

Table 1: Variation of the mean and coefficient of variation of the quality factor with respect to the coefficient of variation of Young's modulus.

Method	CoV(E) [%]	Mean(Q) [−]	σ(Q) [−]	CoV(Q) [%]	t^*_{CPU} [−]
MC	6	13035	980	7.52	2005
PSFEM 1st	6	12967	971	7.49	1.02
PSFEM 2nd	6	13037	971	7.45	1.16
PSFEM p2nd	6	13069	971	7.43	1.04
MC	10	13181	1720	13.05	5015
PSFEM 1st	10	12967	1619	12.49	1.02
PSFEM 2nd	10	13161	1619	12.30	1.16
PSFEM p2nd	10	13250	1619	12.22	1.04
MC	20	13895	4313	31.05	10062
PSFEM 1st	20	12967	3238	24.97	1.02
PSFEM 2nd	20	13744	3238	23.56	1.16
PSFEM p2nd	20	14099	3238	22.97	1.04

NSTI-Nanotech 2007, www.nsti.org, ISBN 1420061844 Vol. 3, 2007