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Summary. This paper presents a general methodology to predict the dynamics of geometrically nonlinear Micro/Nano Electro-Mechanical Systems (M/NEMS) with piezoelectric and dielectric transducers, modelled as laminated thin structures. Modal Reduced Order Models (ROM) are built using finite-element software thanks to a non-intrusive strategy. The resulting system of coupled oscillators is solved with the Harmonic Balance Method (HBM) coupled to an Asymptotic Numerical Method (ANM). The present study focuses on the computation of the ROM, that include the geometrical nonlinear terms and the direct and converse electromechanical couplings. Then, frequency responses and nonlinear modes, including possible internal resonances, are proposed for some particular beams and circular plates M/NEMS architectures.

Keywords: Geometrical nonlinearities, electromechanical coupling, piezoelectric, dielectric, M/NEMS, finite elements.

1 Introduction

Geometrical nonlinearities, due to large transverse displacements of thin structures, are involved in a large range of applications. Among them, Micro-Electro Mechanical Systems (MEMS) developments has been the focus of numerous studies, whose purpose is to master and use the geometrically nonlinear behaviour (among others, see [7, 11, 14, 17]). Recent advances in non-intrusive reduced-order finite element modeling of nonlinear geometric structures offer new perspectives for massive nonlinear prediction in structural computation [8]. An application on piezoelectric nanobridges of such a method has been proposed in [6], with a home made finite element code. The purpose of this paper is to extend this approach to a wider range of MEMS architectures with thin geometries, including beams with complex cross section [16] and laminated beams/plate structures [2, 4, 5].

Two examples of structures are shown on Fig. 1. They are both constituted of a base structure (a silicon / silicon oxide stack) which has been etched through the material to pattern a beam/plate thin structure, with clamped boundary conditions. The electromechanical transducers are constituted of multilayer stacks of an active layer surounded by two electrodes (top and bottom). On Fig. 1, both structures are equipped with two transducers (one at each end of the clamped/clamped beam; an annular one at the edge of the circular plate and another circular one at its center). The structures are at a nanometer (thickness of $\simeq 350$ nm for the beam) or micrometer (thickness $\simeq 2.5$ μm for the plate) scale, with a thin geometry (aspect ratio of 0.012: $0.35/30$ for the beam and $2.5/200$ for the plate). Two electromechanical transduction schemes are considered. The first one is the well known piezoelectric material, and the second one is based on the use of dielectric layers, as introduced in [5]. In this latter case, the excitation results from the electrostatic force created between the charged electrodes which causes a transverse deformation of the dielectric film and a bending of the multilayer structure; the detection of the vibration is capacitive, based on the fluctuation of the capacitance due to the deformation of the dielectric film. In the case of thin layers, both effects can be modelled in the same way [13]. The modelling proposed here thus includes: (i) the geometrical nonlinearities (ii) the laminated structure and (iii) the electromechanical transduction with both converse and direct effects.

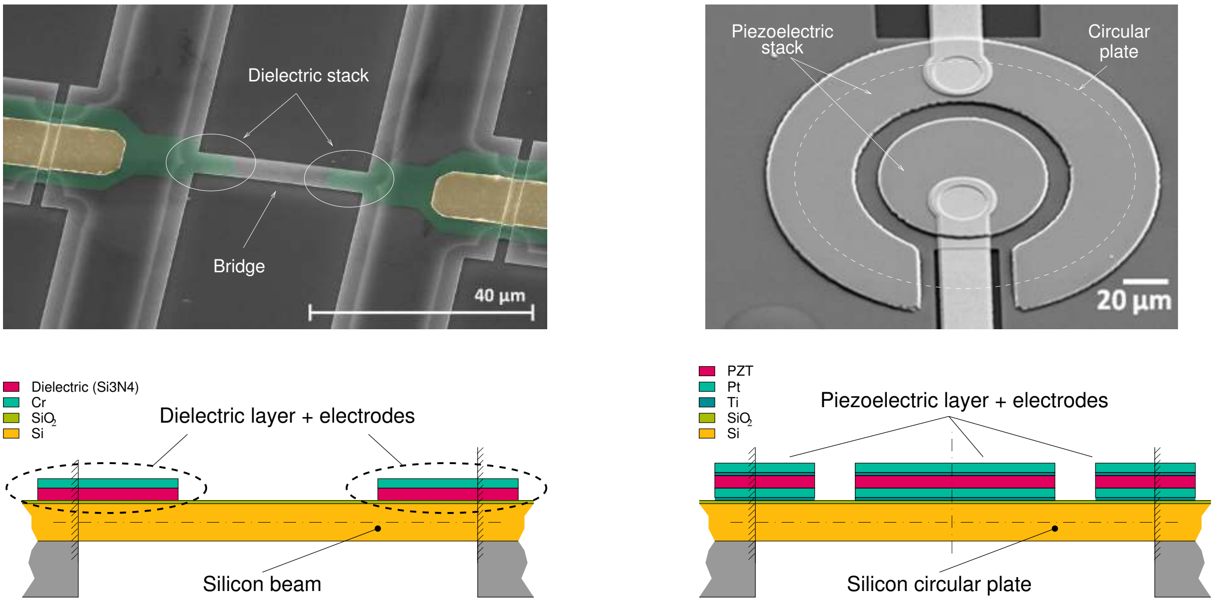

Figure 1. Scanning Microscope Images and cutaway view of some M/NEMS devices: a clamped/clamped beam and a clamped circular plate. Beam dimensions: 5×30 μm, thickness 320 nm, dielectric stack thickness: 35 nm. Plate dimensions: diameter 200 μm, thickness 1 μm, piezoelectric stack thickness: 1.6 μm

2 Finite element reduced-order model

We consider an elastic structure equipped with $P \in \mathbb{N}^*$ thin transducers composed of multilayer stacks including an active layer (piezoelectric/dielectric, Fig. 1). Following the ideas of [12] for the linear case and [6] for the case with geometrical nonlinearities, the governing equations can be written:

$$\begin{cases} \boldsymbol{M}_m\ddot{\boldsymbol{U}} + \boldsymbol{K}_m\boldsymbol{U} + \boldsymbol{f}_{nl}(\boldsymbol{U}) + \displaystyle\sum_{p=1}^{P}\left[\boldsymbol{f}_c^{(p)} + \boldsymbol{P}_c^{(p)}\boldsymbol{U}\right]V^{(p)} = \boldsymbol{F}, & \text{(1a)} \\ C^{(p)}V^{(p)} - \left[\boldsymbol{f}_c^{(p)} + \boldsymbol{P}_c^{(p)}\boldsymbol{U}\right]^{\mathrm{T}}\boldsymbol{U} = Q^{(p)}, \qquad \forall p \in \{1, \dots P\}. & \text{(1b)} \end{cases}$$

In the above equations, $\boldsymbol{U}$ is the vector containing the mechanical degrees of freedom (of size N), $\boldsymbol{F}$ is the mechanical forcing vector (of size N), $V^{(p)}$ is the voltage applied to the p-th. active layer and $Q^{(p)}$ is the electric charge contained in one of its electrodes. $\boldsymbol{M}_m$ and $\boldsymbol{K}_m$ are the mechanical mass and stiffness matrices (of size $N \times N$), $\boldsymbol{f}_{nl}(\boldsymbol{U})$ is the nonlinear part of the internal mechanical forces vector (coming from the geometrical nonlinearities, of size N). All those mechanical quantities are related to the structure with all active layers short-circuited ($V^{(p)} = 0\ \forall p$). $C^{(p)}$ is the electrical capacitance of the p-th. active layer with the elastic structure in blocked state ($\boldsymbol{U} = \boldsymbol{0}$). Finally, $\boldsymbol{f}_c^{(p)}$ is the electromechanical forcing vector (the one introduced in [12], of size N), which couples the p-th active layer to the mechanical dofs and $\boldsymbol{P}_c^{(p)}$ is an electromechanical coupling matrix, related to the geometrical nonlinearities, responsible in particular of parametric excitation effects in thin structures [14].

As shown in [6], we consider $K < N$ eigenmodes $(\boldsymbol{\Phi}_k, \omega_k)$ of the structure with all active layers short circuited ($V^{(p)} = 0\ \forall p$). They are solution of:

$$\left(\boldsymbol{K}_m - \omega^2\boldsymbol{M}_m\right)\boldsymbol{\Phi} = \boldsymbol{0}. \tag{2}$$

and normalized with respect to the mass matrix:

$$\boldsymbol{\Phi}_k^{\mathrm{T}}\boldsymbol{M}_m\boldsymbol{\Phi}_k = 1 \quad \forall k \tag{3}$$

The displacement $\boldsymbol{U}(t)$ is written:

$$\boldsymbol{U}(t) = \sum_{k=1}^{K}\boldsymbol{\Phi}_k q_k(t), \tag{4}$$

with the modal coordinate $q_k(t)$ that verify:

$$\begin{cases} \ddot{q}_k + 2\xi_k\omega_k\dot{q}_k + \omega_k^2 q_k + \sum_{i,j=1}^{K} \beta_{ij}^k q_i q_j + \sum_{i,j,l=1}^{K} \gamma_{ijl}^k q_i q_j q_l \\ \qquad + \sum_{p=1}^{P} \chi_k^{(p)} V^{(p)} + \sum_{p=1}^{P}\sum_{i=1}^{N} \Theta_{ik}^{(p)} q_i V^{(p)} = F_k, \qquad \forall k = 1, \dots K & \text{(5a)} \\ C^{(p)}V^{(p)} - \sum_{k=1}^{K} \chi_k^{(p)} q_k - \sum_{i,j=1}^{K} \Theta_{ij}^{(p)} q_i q_j = Q^{(p)}, \qquad \forall p = 1, \dots P & \text{(5b)} \end{cases}$$

The idea of a non-intrusive method is to use the standard static and modal analyses procedures of finite-elements commercial codes to evaluate the coefficients of the above reduced order model, especially β_{ij}^k, γ_{ijl}^k, $\chi_k^{(p)}$ and $\Theta_{ik}^{(p)}$.

As explained in [9], the nonlinear stiffness coefficients β_{ij}^k and γ_{ijl}^k are computed by prescribing a series of displacement expanded to some linear modes, evaluating nonlinear direct static problems and solving an algebraic linear system. For the electromechanical coupling coefficients $\chi_k^{(p)}$ and $\Theta_{ik}^{(p)}$, several strategies are tested. The first one is to use a standard elastic finite-elements code and to use a thermal analogy: prescribing a given voltage V is equivalent, to some assumptions, to prescribe a given temparature field. It enables in a straighforward manner to compute the linear coefficients $\chi_k^{(p)}$. The nonlinear ones $\Theta_{ij}^{(p)}$ can be evaluated with the same method, the only difference being that the displacement fields result from a geometrically nonlinear thermoelastic static problem. Another one is to use a finite element code with piezoelectric finite elements and geometrical nonlinearities.

3 Computation of frequency responses

The obtained reduced order model (5) can be treated in several manners. If it is reduced to very few oscillators (with normal form for instance [15]), analytical perturbation methods can be used (see [10]). Here, we are interested in numerical methods, which enables to consider more oscillators in (5) and compute accurately frequency responses. We use here a combination of the Harmonic Balance Method (HBM), to compute periodic solutions, and an Asymptotic Numerical Method (ANM) to follow the solution branches [1, 3]. It requires to rewrite (5) in the state space and under a quadratic form, which is done by introducing the modal velocities $v_k = q_k$ and new slave variables $S_{ij} = q_i q_j$.

We compute frequency responses, when the structure is subjected to an harmonic forcing (for instance by prescribing the voltage in one of the transducer stacks $V(t) = V_0 \cos \Omega t$) or nonlinear modes, which correspond to the periodic solutions of Eq. (5) in free/conservative vibrations. The latter case conducts to compute backbone curves, which are very interesting in practice since they constitute the skeleton of the forced vibrations responses. However, since the system is conservative in this case, numerous internal resonances are computed which increases the computation time. An example is shown on Fig. 2 on which some responses of a homogeneous isotropic circular plate are presented. The four first NNM have been computed by assuming that the axisymmetric and asymmetric problems are separated. Numerous modal interactions at high vibration amplitudes are obtained, for which harmonics of order $3, 7, 9, 10$ emerge in the free response of the plate around the first mode. The asymmetric modes are subject to a 1:1 internal resonance, well computed by the algorithm.

References

[1] R. Arquier, S. Karkar, A. Lazarus, O. Thomas, C. Vergez, and B. Cochelin. Manlab 2.0: an interactive path-following and bifurcation analysis software. Technical report, Laboratoire de Mcanique et d'Acoustique, CNRS, http://manlab.lma.cnrs-mrs.fr, 2005-2011.

[2] C. Ayela, L. Nicu, C. Soyer, É. Cattan, and C. Bergaud. Determination of the d_{31} piezoelectric coefficient of $pbzr_x ti_{1-x} o_3$ thin films using multilayer buckled micromembranes. *Journal of Applied Physics*, 100:054908, 2006.

[3] B. Cochelin and C. Vergez. A high order purely frequential harmonic balance formulation. *Journal of Sound and Vibration*, 324(1-2):243–262, 2009.

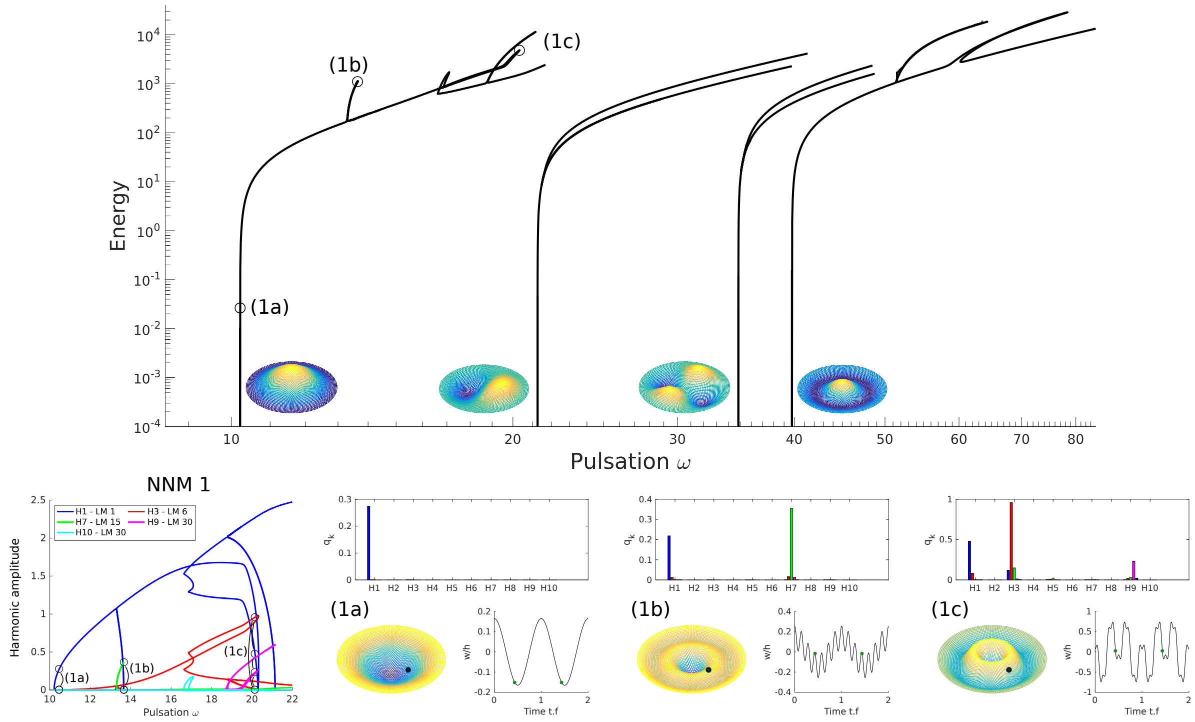

Figure 2. Nonlinear modes of an elastic clamped circular plate.

[4] D. Dezest, O. Thomas, F. Mathieu, L. Mazenq, C. Soyer, J. Costecalde, D. Remiens, J.-F. Deü, and L. Nicu. Wafer-scale fabrication of self-actuated piezoelectric nanoelectromechanical resonators based on lead zirconate titanate (pzt). *Journal of Micromechanics and Microengineering*, 25(3):035002, 2015.

[5] C. Fuinel, K. Daffé, A. Laborde, O. Thomas, L. Mazenq, L. Nicu, T. Leichlé, and B. Legrand. High-K thin films as dielectric transducers for flexural M/NEMS resonators. In *Proc. of the 29th. IEEE international conference on micro electro mechanical systems (MEMS 2016) conference*, Shanghai, China, January 2016.

[6] A. Lazarus, O. Thomas, and J.-F. Deü. Finite elements reduced order models for nonlinear vibrations of piezoelectric layered beams with applications to NEMS. *Finite Elements in Analysis and Design*, 49(1):35–51, 2012.

[7] M. H. Matheny, L. G. Villanueva, R. B. Karabalin, J. E. Sader, and M. L. Roukes. Nonlinear mode-coupling in nanomechanical systems. *Nano Letters*, 13(4):1622–1626, 2013.

[8] M. P. Mignolet, A. Przekop, S. A. Rizzi, and S. M. Spottswood. A review of indirect/non-intrusive reduced order modeling of nonlinear geometric structures. *Journal of Sound and Vibration*, 332(10):2437–2460, 2013.

[9] A. A. Muravyov and S. A. Rizzi. Determination of nonlinear stiffness with application to random vibration of geometrically nonlinear structures. *Computers and Structures*, 81(15):1513–1523, 2003.

[10] A. H. Nayfeh and D. T. Mook. *Nonlinear oscillations*. John Wiley & sons, inc., New-York, 1979.

[11] O. Shoshani, D. Heywood, Y. Yang, T. W. Kenny, and S. W. Shaw. Phase noise reduction in an mems oscillator using a nonlinearly enhanced synchronization domain. *Lournal of Microelectromechanical Systems*, 25(5):870–876, 2016.

[12] O. Thomas, J.-F. Deü, and J. Ducarne. Vibration of an elastic structure with shunted piezoelectric patches: efficient finite-element formulation and electromechanical coupling coefficients. *International Journal of Numerical Methods in Engineering*, 80(2):235–268, 2009.

[13] O. Thomas, B. Legrand, and C. Fuinel. Optimization of length and thickness of smart transduction layers on beam structures for control and m/nems applications. In *Proceedings of SMASIS 2015 (ASME 2015 Conference on Smart Materials Adaptive Structures and Intelligent Systems*, Colorado Springs, USA, September 2015. Paper 8857.

[14] O. Thomas, F. Mathieu, W. Mansfield, C. Huang, S. Trolier-McKinstry, and L. Nicu. Efficient parametric amplification in mems with integrated piezoelectric actuation and sensing capabilities. *Applied Physics Letters*, 102(16):163504, 2013.

[15] C. Touzé, O. Thomas, and A. Chaigne. Hardening/softening behaviour in non-linear oscillations of structural systems using non-linear normal modes. *Journal of Sound Vibration*, 273(1-2):77–101, 2004.

[16] L. G. Villanueva, R. B. Karabalin, M. H. Matheny, D. Chi, J. E. Sader, and M. L. Roukes. Nonlinearity in nanomechanical cantilevers. *Physical Review B*, 87:024304, 2013.

[17] L. G. Villanueva, E. Kenig, R. B. Karabalin, M. H. Matheny, R. Lifshitz, M. C. Cross, and M. L. Roukes. Surpassing fundamental limits of oscillators using nonlinear resonators. *Physical Review Letters*, 110(17):177208, 2013.