The Origin of Mass-change Sensitivity within Piezoelectrically-actuated Millimeter-sized Cantilever (PEMC) sensors: Vibrational Analysis through Experiment and Finite Element Modeling

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Abstract:

A 3D finite element model (FEM) of the PEMC sensor was developed to characterize the modes of vibration that have demonstrated high sensitivity to mass-change in experimentally fabricated sensors. The fundamental bending mode of vibration and the 1st bending harmonic are predicted at 10.0 kHz and 86.8 kHz, respectively, within approximately 5 % of the experimentally measured resonances. Low order torsional modes of vibration are predicted by mechanical simulation, but remain electrically unobservable by means of impedance characterization in both experimentally fabricated sensors and the FEM frequency response analysis. The cantilever also undergoes combinations of extension, buckling, and lateral modes of vibration in the higher order region of the frequency spectrum. These higher order modes also give rise to electrically observable resonances in the experimentally measured spectrum and the FEM frequency response spectrum based on impedance characterization.

Keywords: piezoelectric, cantilever, composite, sensitivity, frequency response

Introduction

The PEMC sensor is a multi-layered, composite cantilever of non-uniform cross-section. It consists of piezoelectric, polymer, and borosilicate glass layers (figure 1). Acting as both sensor and actuator, the harmonically driven resonator exhibits modes of vibration that are highly sensitive to mass-changes induced by the binding of a biological or chemical target to the functionalized cantilever surface (i.e. a recognition event). Applications of the PEMC sensor have been demonstrated with respect to the detection of environmental [1] and food-borne pathogens [2, 3], biological warfare agents

[4, 5], immunoassay [6], genomics [7], and proteomics [8] in both gas and liquid. Extension to complex food-media [2, 3], cell-culture [9], and bodily fluid settings [6] have also been demonstrated. Sensitivity to mass-change has been demonstrated using the fundamental modes of vibration, but focus has turned towards utilizing the higher order resonant modes since their sensitivity is higher relative to their lower order counterparts.



Figure 1- Schematic diagram of the PEMC sensor and the corresponding electrical and mechanical boundary conditions.

Theory

Cantilever Beam Mechanics:

The composite PEMC sensor is assumed to be governed by Euler-Bernoulli (E.B.) Beam Theory since the length to thickness ratio is much greater than unity. Equation 1 presents the 1-D time-dependent E.B. beam equation for a driven cantilever beam, where u is the displacement, E is the modulus of elasticity, I is the area moment of inertia, and f(t) is the forcing function (i.e. the applied load).

$$\frac{\partial^2}{\partial x^2} \left(EI \frac{\partial^2 u}{\partial x^2} \right) = f(t) \tag{1}$$

A full description of the composite cantilever beam requires the solution of the beam equation for each domain coupled through boundary conditions. Thus, analysis of a composite cantilever becomes increasingly complicated, especially when one of the domains is electromechanically coupled. Therefore, the finite element method is suited towards the analysis of these types of structures.

Piezoelectric Theory:

Since the cantilever beam is made of piezoelectric material, electrical and mechanical effects are coupled. This coupling is illustrated by the form of the piezoelectric constitutive relationships given in equations 2 and 3, where σ is the stress matrix, ε is the strain matrix, E is the applied electric field vector, e is the piezoelectric coupling matrix, c is the elasticity matrix, D is the electric displacement vector, and ϵ is the relative permittivity matrix.

$$\sigma = c\varepsilon - e^T E \tag{2}$$

$$D = e\varepsilon + \epsilon E \tag{3}$$

The cantilever is piezoelectrically actuated through a harmonically changing electric field in the direction of the material polarization axis (i.e. the y-direction).

Use of COMSOL Multiphysics

The structural mechanics-piezoelectric module was used to carry out 3D eigenfrequency analysis and 3D frequency response analysis on the PEMC sensor using default Lagrange-Quadratic type elements. Analysis was carried out through the use of global variables representing the integrated normal surface current density (I) and the integrated surface charge density (Q) across the electrode surfaces. The phase angle (θ) obtained through impedance analysis is given by equation 4, where X_L is the inductive reactance, X_{C} is the capacitive reactance, and R is the electrical resistance. *Re* and Im represent the real and imaginary components of the complex quantities I and Q, respectively.

$$\theta = \arctan\left(\frac{lm(l)}{Re(l)}\right) = \arctan\left(\frac{X_L - X_C}{R}\right)$$
 (4)

The electrical impedance (Z) can be calculated by use of equation 5, where V is the applied voltage, and ω is the frequency [10].

$$Z = \frac{V}{I} = \frac{V}{\omega[jRe(Q) - Im(Q)]}$$
(5)

Loss factor damping parameters were employed to account for energy losses within the composite cantilever. The loss factor parameters were also used as fitting parameters to yield quality factors similar to those observed experimentally for the major resonances of interest. Loss factors used in the FEM range between one and five percent.

Experiment

Fabrication:

127 µm thick, type-5A lead zirconate titanate (PZT-5A) was purchased from Piezo Systems, Inc. for use as the piezoelectric domain. The corresponding preloaded PZT-5A material in the COMSOL library was used to model the anisotropic piezoelectric domain for the FEM. The piezoelectric domain has length and width of 2.5 mm and 1 mm, respectively. The silica domain is positioned 0.5 mm from the clamp and has length, width, and thickness dimensions of 2 mm, 1 mm, and 160 µm, respectively. The 30 um thick polymer bonding layer has length and width dimensions equivalent to the silica domain. Material properties consistent with Maraldo and Mutharasan [11] were used for the finite element method material properties. Boundary conditions employed in the model can be found in figure 1.

Experimental Apparatus:

A Hewlett-Packard impedance analyzer was used to obtain the experimentally measured frequency response of the cantilever over a range of 0-2 MHz subject to a 100 mV harmonic driving force. Commercial Labview software was used for remote operation and interfacing of the impedance analyzer-cantilever system.

Results and Discussion

A comparison of the electromechanical simulations carried out using the FEM and the spectrums of experimentally fabricated sensors reveals that the composite cantilever contains bending, torsional, extension, buckling, and lateral modes of vibration. The experimentally measured frequency response spectrum and the spectrum obtained from the FEM frequency response analysis (see Theory section) are presented in figures 2 and 3, respectively.







Figure 3- Frequency response obtained using the 3D finite element model over a range of 0 - 2 MHz.

Within the higher order harmonics of the eigenfrequency spectrum (approximately 500-1,000 kHz), electrically observable modes (i.e. modes observable by means of impedance characterization) exist that have high sensitivity to mass-change. As the cantilever undergoes higher order resonance, some modes within the composite structure exhibit both harmonic and anharmonic coupling of the vibrations between the composite layers of the structure. The origin of the electrically observable modes in the PEMC sensor, and therefore the experimentally observable modes that demonstrate sensitivity to mass-change, is due to vibrations with bending, extension, and buckling character. In addition, lateral vibrations are electrically observable in the higher order region of the spectrum (approximately 1.5 - 2 MHz), but these modes have not yet been exploited experimentally for detection purposes.

Experiment also reveals that some observable modes are more sensitive to mass-change and damping effects than others, indicating that the sensor exhibits vibrations that interact differently with respect to mass-loading and dissipative effects. Mode shape is observed to have a direct correlation with the degree of electrical observability and sensitivity. In the higher order range, combinations of the aforementioned mode shapes also appear. The frequency response over the range of 0 - 100 kHz is presented in figure 4.



Figure 4- FEM frequency response over the range of 0-100 kHz.

The plot captures the fundamental bending mode and the 1st bending harmonic. One can notice from the mode shapes of the first four modes of vibration (figures 5-8), that the fundamental torsional mode and 1st torsional harmonic are not observable by impedance characterization. This confirms the belief that the PEMC is a bending-mode cantilever sensor in the lower order range of the frequency spectrum.



Figure 5- Fundamental bending mode at 10.0 kHz.



Figure 6- 1st bending harmonic at 86.8 kHz.



Figure 7- Fundamental torsional mode at 53.6 kHz.



Figure 8- 1st torsional harmonic at 60.0 kHz.

Conclusions

In this paper finite element modeling was used to show that the PEMC sensor is a bending mode resonant sensor in the lower order frequency range of the frequency response spectrum. The sensor also displays electrically observable higher order modes of vibration that consist of extension, buckling, and lateral character. Although the sensor possesses mechanical torsional modes of vibration, these modes remain electrically unobservable by means of impedance characterization, and thus, cannot be used for detection unless alterations are made to the sensor to make these modes electrically observable.

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