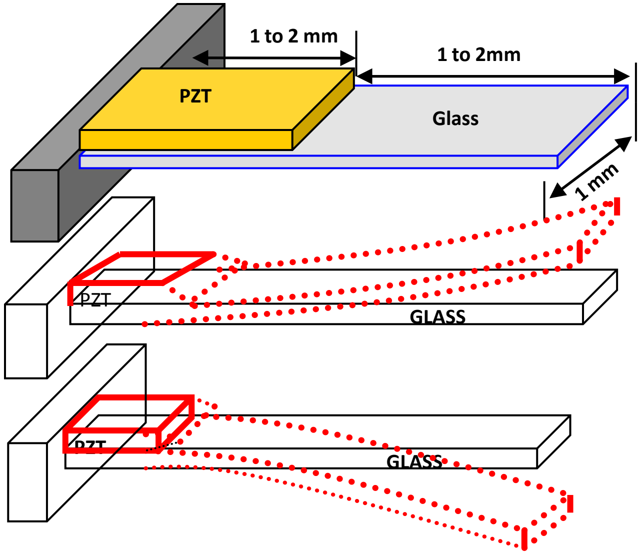
Presented at the COMSOL Conference 2009 Boston

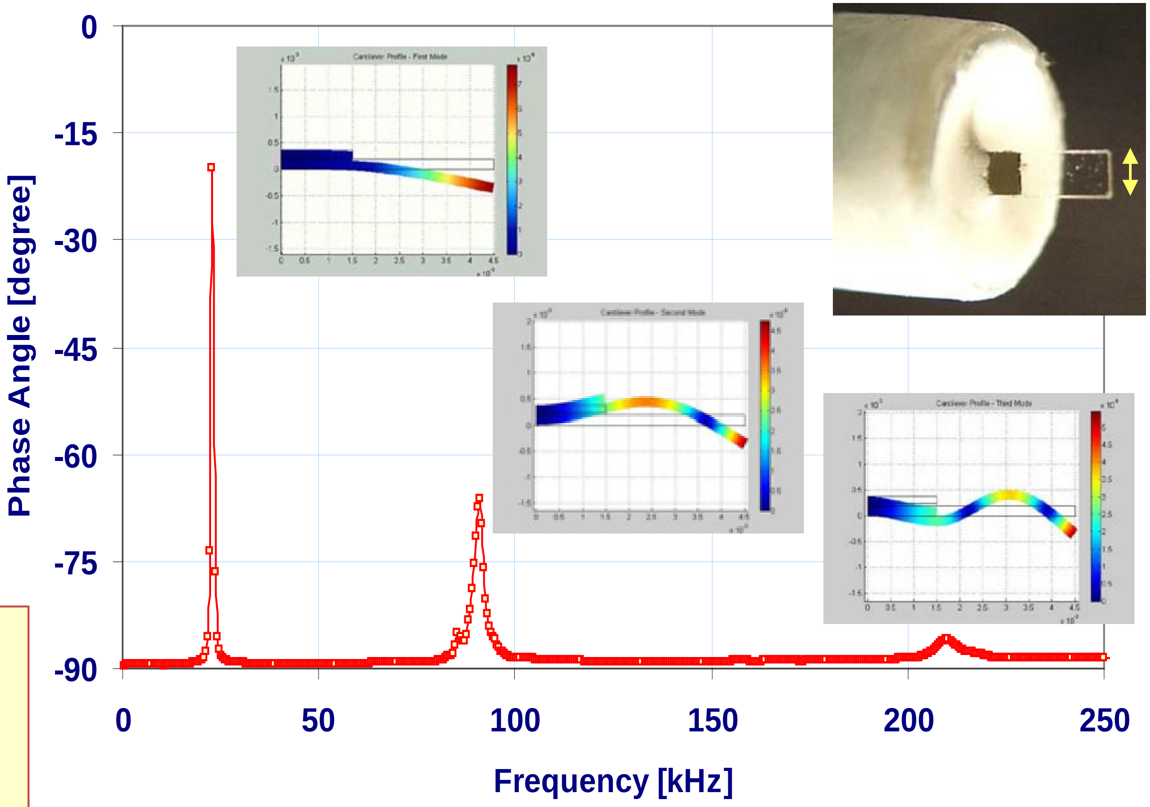
The Origin of Mass-change Sensitivity in PEMC sensors:

Experimental and FEM Vibrational Analysis

Blake Johnson and Raj Mutharasan
Department of Chemical and Biological Engineering
Drexel University
Philadelphia, PA 19104

Piezoelectric-Excited Millimeter-sized Cantilever (PEMC) Sensors





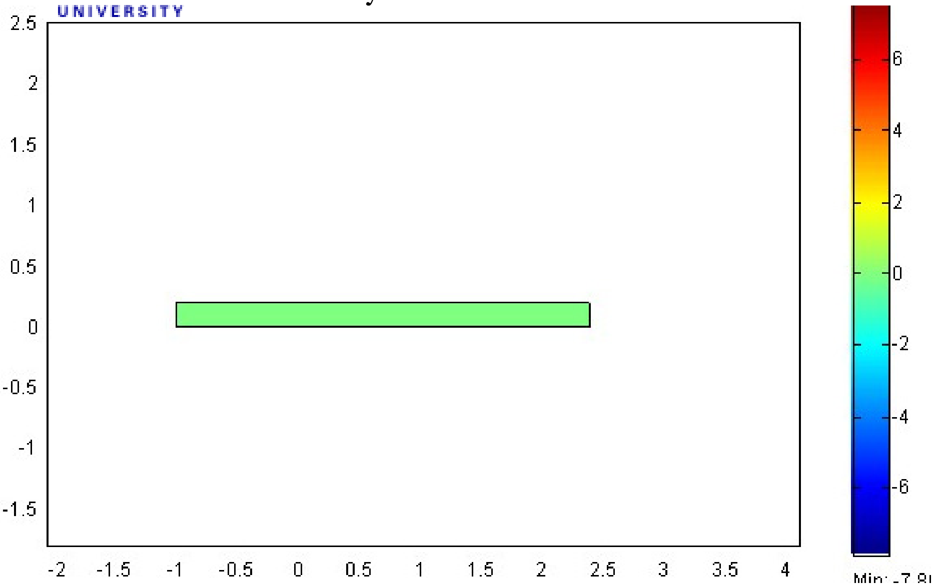
Typical spectrum measured experimentally, we want to predict this behavior.

Sensing Principle

- Resonant frequency depends on cantilever's mass.
- Surface is immobilized with a recognition molecule (eg. Antibody; ssDNA).
- When target attaches to the cantilever, mass changes, and resonant frequency changes.

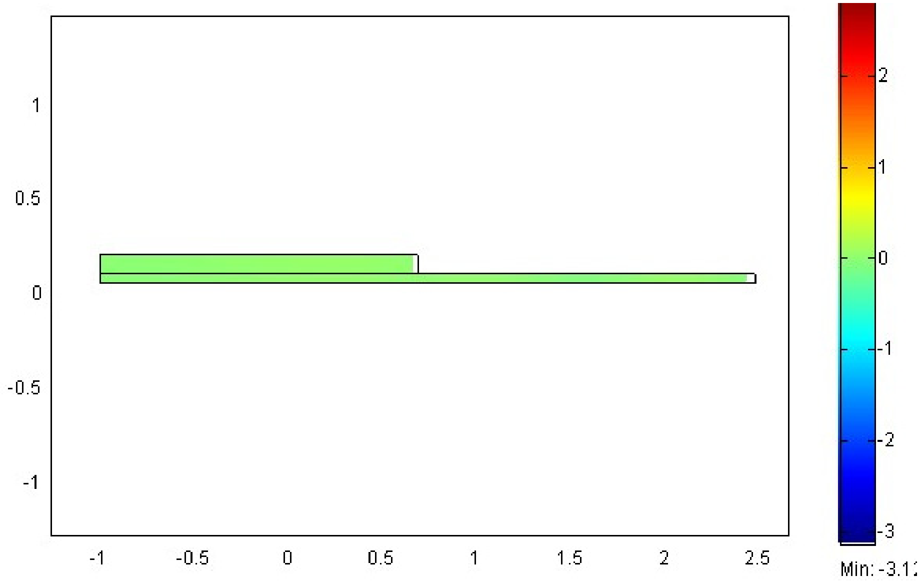
Oscillation characteristics of PEMC Sensors

PZT only – fixed at one end



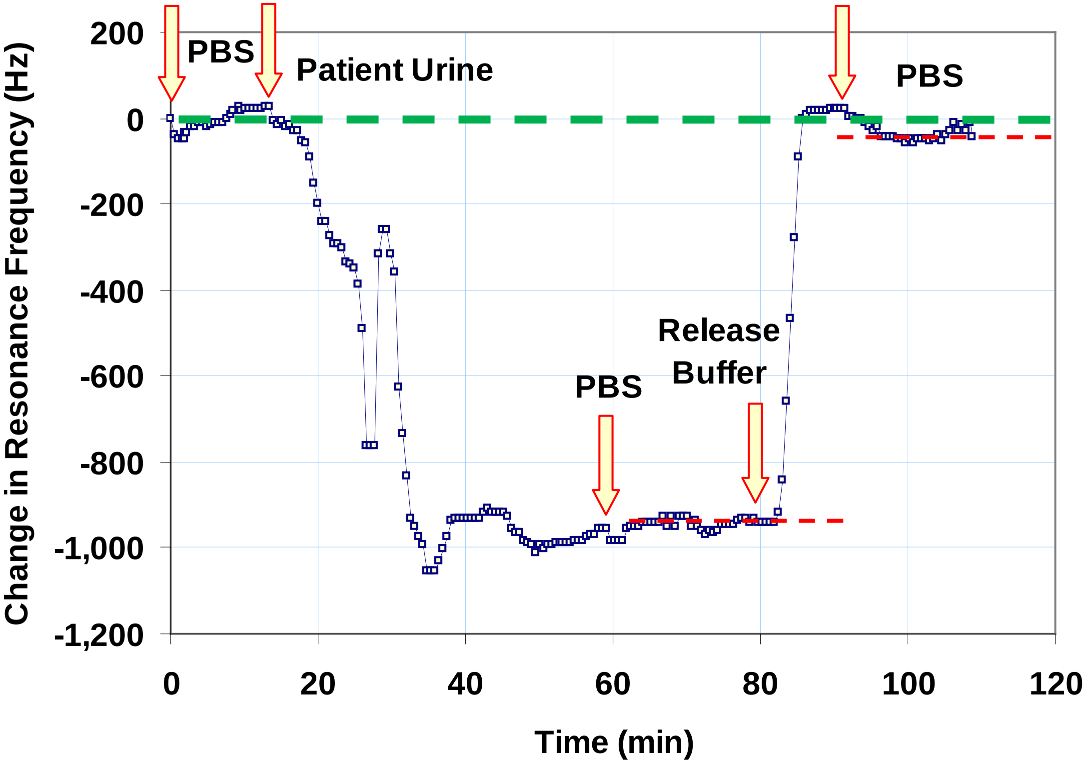

PZT only – fixed at one end
Displacement

PZT-bonded to Low modulus base

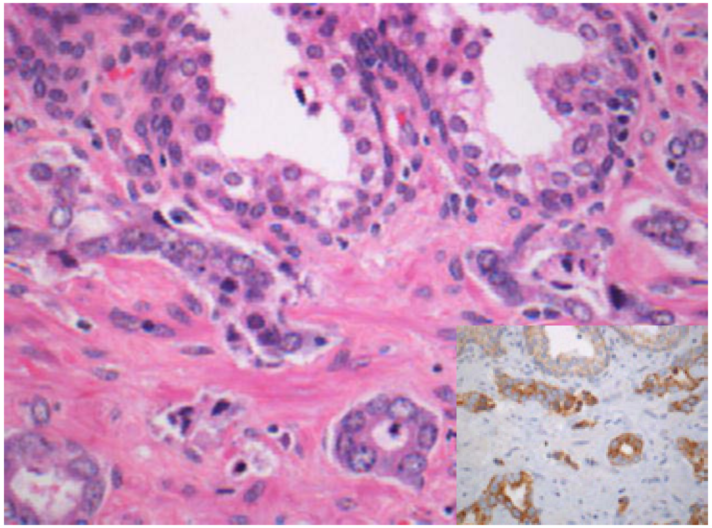


PZT-bonded to High modulus base

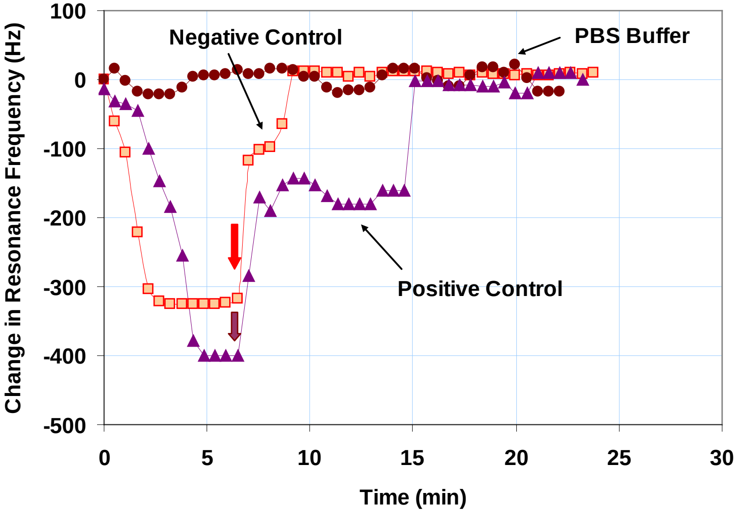
AMACR in patient urine – Patient 3



Prostate cancer biomarker:
α-methylacyl-CoA racemase (AMACR)



Case #	Age	Gleason Score	Post Biopsy Stage	PSA Value	$PEMC_a$ Response	$PEMC_a$ Control Urine
Case 1	61	7	pT2c	11.6 ng/mL	-4,314±35 Hz	10±21 Hz
Case 2	83	6	pT2a	12.6 ng/mL	-269±17 Hz	10±6 Hz
Case 3	64	8	pT2c	78.4 ng/mL	-977±64 Hz	-63±14 Hz
Case 4	59	7	pT2b	4.6 ng/mL	-600±31 Hz	-35±24 Hz
Case 5	65	7	PT2c	2.0 ng/mL	-801±81 Hz	-20±15 Hz



Maraldo, E.; Garcia, R;Mutharasan, R. **2007**. *Analytical Chemistry,* 79 (20): 7683-7690

Notable detection applications and Motivation

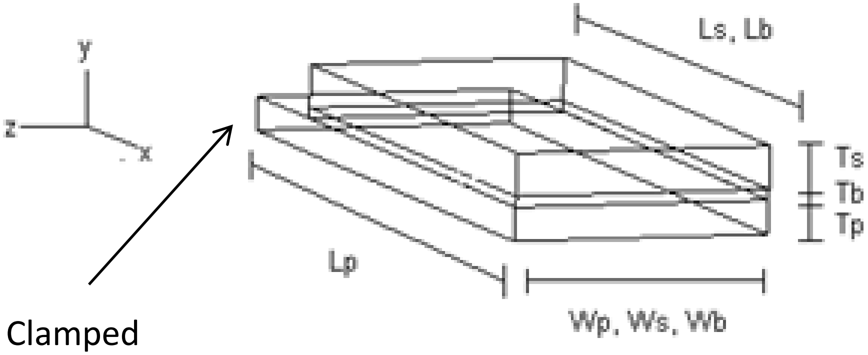
Detection Application	**Sensitivity**
Bacillus anthracis (Anthrax) spores in air	5 spores/L
E. coli O157:H7 in food media	1 cell/mL
Prostate cancer biomarker (AMACR) in urine	2 fg/mL

Motivation:

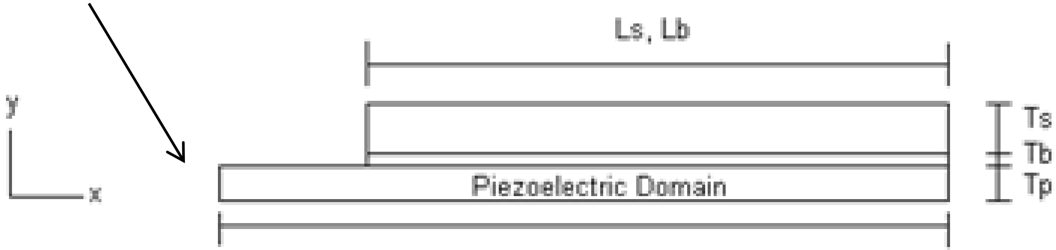
- Vibration characteristics of PEMC sensors are complex and remain unexplored.
- Understand the origin of mass-change sensitivity in PEMC sensors using modeling.
- Use simulation as tool for creation of other sensitive structures.
- Structure the model to simulate the quantities we measure experimentally.

Campbell, C; Mutharasan, R. **2007**. *Biosensors and Bioelectronics*, 23: 1039 – 1045
Campbell, C; Mutharasan, R. **2007**. *Analytical Chemistry*, 79 (3): 1145 – 1152
Campbell, C; Mutharasan, R. **2007**. *Environmental Science and Technology*, 41 (5): 1668 – 1674
Maraldo, D; Garcia, F; Mutharasan, R. **2007**. *Analytical Chemistry,* 79 (20): 7683 - 7690

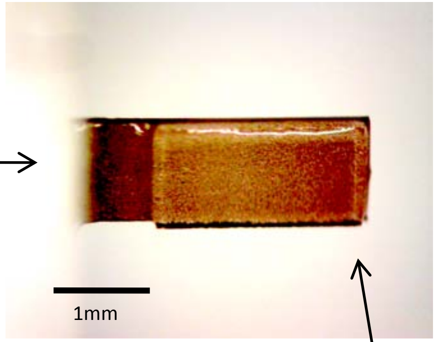
Schematic of PEMC sensor and Experimentally Fabricated Sensor



Clamped edge



Clamped edge



Free edge

Cantilever Dimensions:

- Length (L) ~ 2.5 mm
- Width (W) ~ 1 mm
- Thickness (T) ~ 200 µm

Excitation and Measurement Principle:

- Actuation via harmonic E-field along polarization axis of PZT.
- Inverse piezoelectric effect generates expansion/contraction of the PZT material.
- The resonant frequencies are measurable by the electrical impedance of the piezoelectric domain.

Use of *COMSOL Multiphysics*

COMSOL Modules Used:

- *Structural Mechanics Module*
- *Piezoelectric effects*
- *Piezo Plane Stress*
    - *Damped Eigenfrequency Analysis*
    - *Frequency Response Analysis*
- *Simulations in vacuum*

Piezoelectric Material Constitutive Relations (anisotropic)

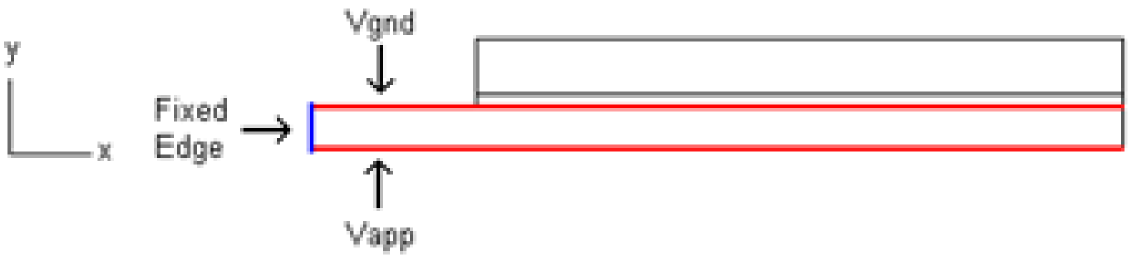
$$\sigma = c\varepsilon - e^T E$$

Electromechanical coupling

$$D = e\varepsilon + \epsilon E$$

Boundary Conditions

- Material polarized in y-direction.
- E-field applied in the y-direction.



Voltage applied = *0.1 sin (ω t)*

Frequency Response Analysis

Scalar potential equation:

$$-\nabla\,(\varepsilon_0\varepsilon_r\nabla V) = \rho_v$$

Quasi-static electric currents equation:

$$-\nabla\,((\sigma_e + j\omega\varepsilon_0\varepsilon_r)\nabla V) = \rho_v$$

Additional expressions employed:

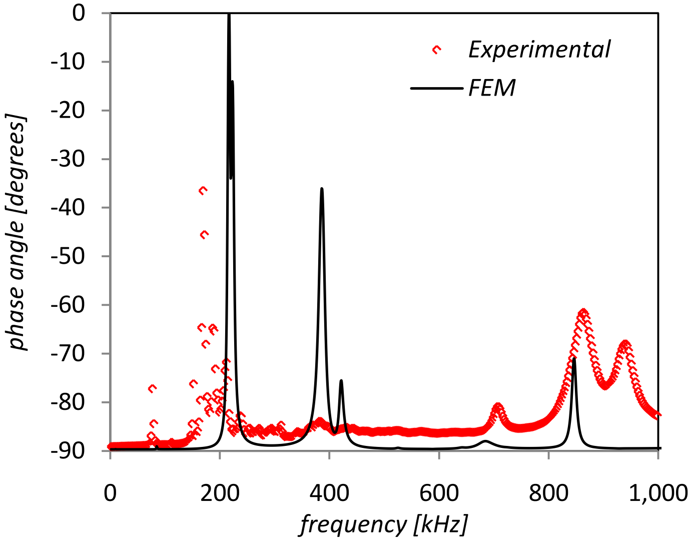
- excitation frequency: *freq_smpz3d*
- electrical impedance: *V/abs(I)*
- phase angle: $\tan^{-1}[Im(I)/Re(I)]$

Loss factor damping:

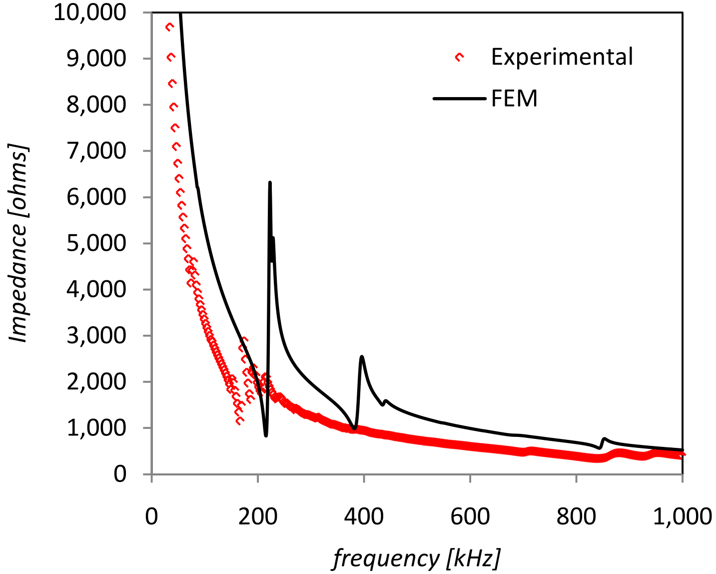
$$G^* = G' + jG'' = (1 + j\eta)G'$$

$$Loss\ Factor = \eta = \frac{G''}{G'}$$

G,G', and G'' are stress relaxation function of viscoelastic material, storage modulus, and loss modulus, respectively.*

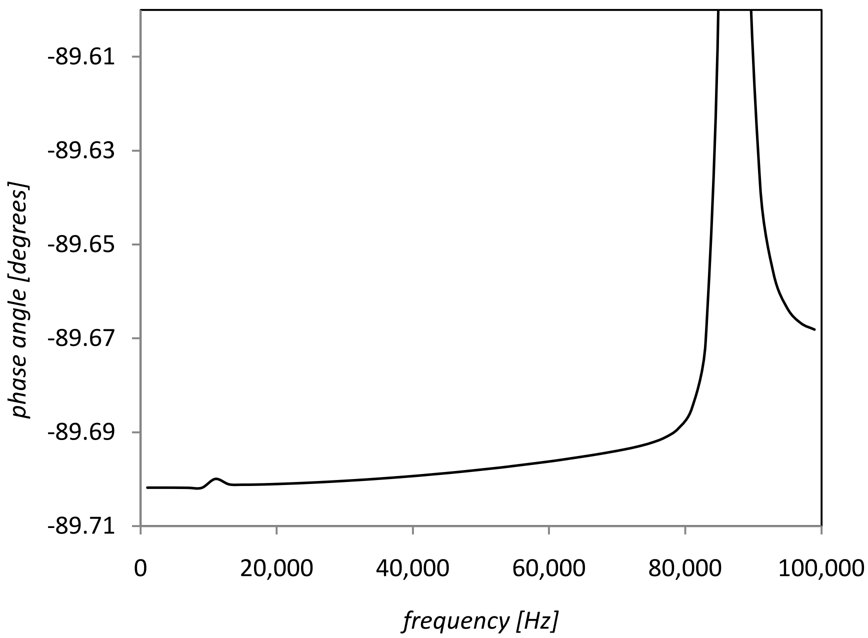


(Simulation time ~ 30 min)



Fundamental Mode Range (0 – 100 kHz):

FEM frequency response analysis



* Contains modes of vibrations sensitive to mass-changes.

* 2nd mode (~80 kHz) used most frequently for detection due to high Q- factor.

* Only 2 resonances in the range of 0 – 100 kHz are electrically measurable using impedance.

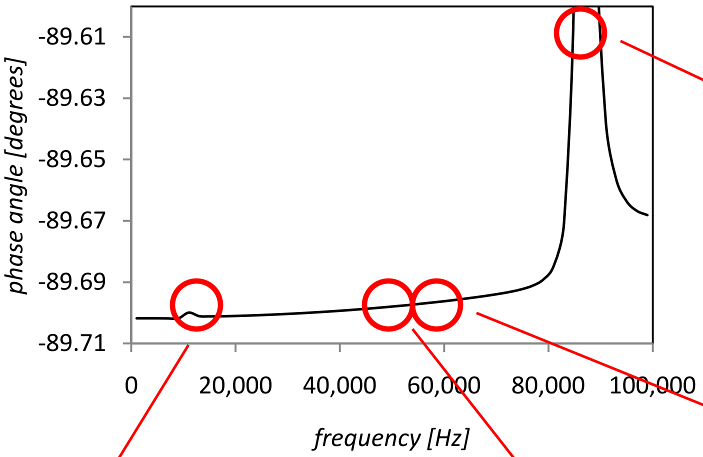
Damped Eigenfrequency Analysis

(Simulation time ~ 1 min)

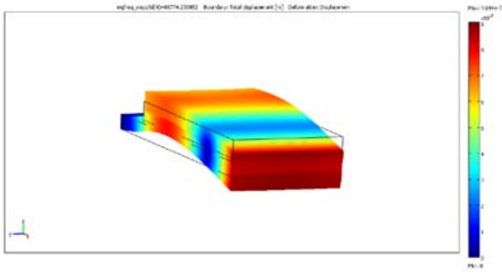
$$M\ddot{U} + K\,U = F$$

$$\omega^2 = M^{-1}K$$

$$f_n = k_n\sqrt{\frac{K}{M_e}}$$



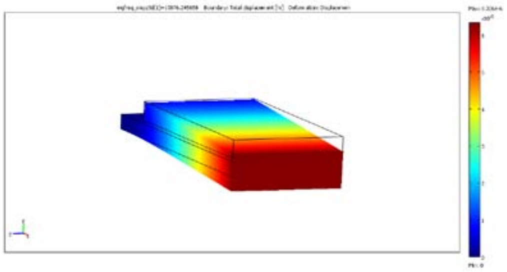
Electrically Observable



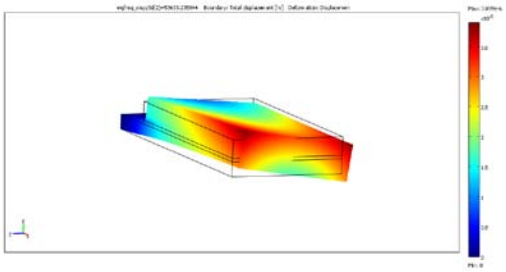
2nd bending mode (86.8 kHz)

Electrically Observable

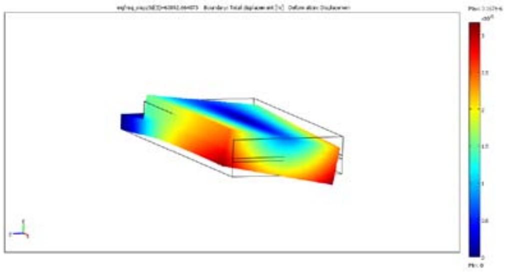
Not electrically observable



Fundamental bending mode (10.0 kHz)



Fundamental torsional mode (53.6 kHz)



2nd torsional mode (60.0 kHz)

Summary

- Used *COMSOL Multiphysics* to simulate the frequency response of the PEMC sensor by impedance characterization.
- Simulation qualitatively predicts the experimentally measured frequency response.
- Assessed the lower order modes of vibration that have been used experimentally for detection using *COMSOL's* eigenfrequency analysis.
- PEMC sensor is sensitive in the bending mode.
- Torsional modes of vibration do not give rise to electrically observable resonances using impedance characterization.

Recommendations

- Recommendations to *COMSOL Multiphysics* developers
  - *Modeling of nonlinear stress-strain material effects.*
  - *Modeling of nonlinear piezoelectric effects.*
  - *Addition of more realistic damping models.*

- Acknowledgements
  - *Advisor: Dr. Raj Mutharasan*
  - *This work was made possible by National Science Foundation Grant CBET-0828987.*