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

**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.

Typical spectrum measured experimentally, we want to predict this behavior.
Oscillation characteristics of PEMC Sensors

PZT only – fixed at one end

PZT-bonded to Low modulus base

PZT only – fixed at one end
Displacement

PZT-bonded to High modulus base

PZT-bonded to Low modulus base

PZT-bonded to High modulus base
## Prostate cancer biomarker: 
**α-methylacyl-CoA racemase (AMACR)**

### Case 1
- **Age:** 61
- **Gleason Score:** 7
- **Post Biopsy Stage:** pT2c
- **PSA Value:** 11.6 ng/mL
- **PEMC<sub>a</sub> Response:** -4314±35 Hz
- **PEMC<sub>a</sub> Control Urine:** 10±21 Hz

### Case 2
- **Age:** 83
- **Gleason Score:** 6
- **Post Biopsy Stage:** pT2a
- **PSA Value:** 12.6 ng/mL
- **PEMC<sub>a</sub> Response:** -269±17 Hz
- **PEMC<sub>a</sub> Control Urine:** 10±6 Hz

### Case 3
- **Age:** 64
- **Gleason Score:** 8
- **Post Biopsy Stage:** pT2c
- **PSA Value:** 78.4 ng/mL
- **PEMC<sub>a</sub> Response:** -977±64 Hz
- **PEMC<sub>a</sub> Control Urine:** -63±14 Hz

### Case 4
- **Age:** 59
- **Gleason Score:** 7
- **Post Biopsy Stage:** pT2b
- **PSA Value:** 4.6 ng/mL
- **PEMC<sub>a</sub> Response:** -600±31 Hz
- **PEMC<sub>a</sub> Control Urine:** -35±24 Hz

### Case 5
- **Age:** 65
- **Gleason Score:** 7
- **Post Biopsy Stage:** PT2c
- **PSA Value:** 2.0 ng/mL
- **PEMC<sub>a</sub> Response:** -801±81 Hz
- **PEMC<sub>a</sub> Control Urine:** -20±15 Hz

---

### Notable detection applications and Motivation

<table>
<thead>
<tr>
<th>Detection Application</th>
<th>Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>Bacillus anthracis</em> (Anthrax) spores in air</td>
<td>5 spores/L</td>
</tr>
<tr>
<td><em>E. coli</em> O157:H7 in food media</td>
<td>1 cell/mL</td>
</tr>
<tr>
<td>Prostate cancer biomarker (AMACR) in urine</td>
<td>2 fg/mL</td>
</tr>
</tbody>
</table>

**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

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.

Cantilever Dimensions:

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

\[ \sigma = c_{ij} \varepsilon_{ij} - e_i^T E \]

Electromechanical coupling

\[ D = \varepsilon_{ij} \varepsilon_{ij} + \varepsilon E \]

**Boundary Conditions**

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

Voltage applied = 0.1 \( \sin (\omega t) \)
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: \textit{freq\_smpz3d}
- electrical impedance: \(V/\text{abs}(I)\)
- phase angle: \(\tan^{-1}[\text{Im}(I)/\text{Re}(I)]\)

Loss factor damping:

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

\[\text{Loss Factor} = \eta = \frac{G''}{G'}\]

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

(Simulation time \(\sim 30\) min)
Fundamental Mode Range 
(0 – 100 kHz):

* Contains modes of vibrations sensitive to mass-changes.

* 2\textsuperscript{nd} 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

\[ M \ddot{U} + K U = F \]

\[ \omega^2 = M^{-1}K \]

\[ f_n = k_n \frac{\sqrt{K}}{\sqrt{M}} \]

Fundamental bending mode (10.0 kHz)  
Fundamental torsional mode (53.6 kHz)  
2nd torsional mode (60.0 kHz)  

Simulation time ~ 1 min

2nd bending mode (86.8 kHz)  

Electrically Observable  
Not electrically observable

COMSOL Conference- Boston 2009
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.