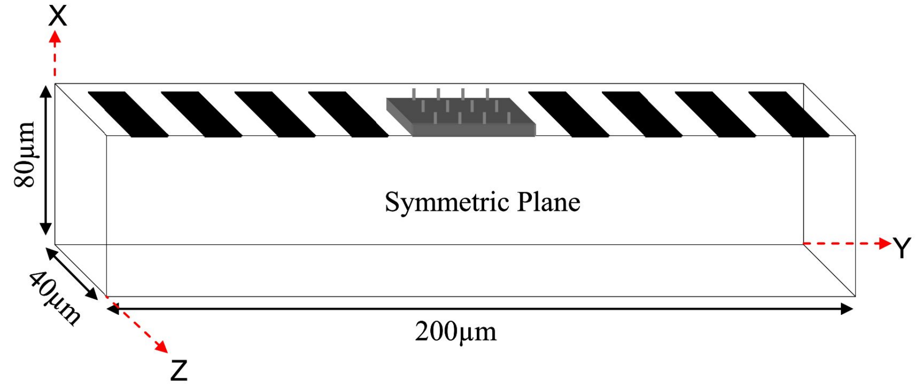
Model Development



Schematic representation of the SAW sensor

- **XY Lithium Niobate (200μm x 80μm x 40 μm) is the piezoelectric substrate where Y is the wave propagation direction.**
- **Interdigitated transducers (10 μm width x 10 μm spacing) are treated as massless conductive boundaries.**
- **Gold square nanopillars (100nm width x 1μm height) are placed on top of the gold active layer (20μm x 20μm x 1 μm).**
- **Sensor performance is evaluated before and after 100nm PMMA adsorption (represents anylate adsorption).**

Modeling Approach

- **Input – Two types of wave perturbation was used:**
  - **Impulse wave function**

$$V_{i+} = \begin{cases} +0.5V, t \le 1ns \\ 0V, t > 1ns \end{cases}, V_{i-} = \begin{cases} -0.5V, t \le 1ns \\ 0V, t > 1ns \end{cases}$$

where V_{i+} and V_{i-} were applied to the alternate fingers of the generator IDT

  - **Sinusoidal wave function**

$$V_i = 1 \times \sin(2\pi \times f \times t), f = 100MHz, t = 100ns$$

where V_i is applied to the alternate fingers of the generator IDT while the others are grounded

- **Output – voltage at the alternate fingers of the receiver IDT is measured and the insertion loss is calculated by taking the ratio of output signal to input**

$$IL = 20 \times \log_{10} \left| \frac{v_{output}}{v_{input}} \right| (dB)$$

- **Sensitivity – The differential signal attenuation per unit mass loading is determined as a measure of detection sensitivity**

Governing Equations

- **Acoustic wave propagation is governed by Gauss law for its electrical behavior and Newton's law for its mechanical behavior.**

$$T = C^E \bullet S - e \bullet E \qquad D = e \bullet S + \varepsilon^s \bullet E$$

$$\nabla \bullet [e \bullet \nabla \varphi] + \nabla \bullet [C^E \bullet \nabla_s u] - \rho \ddot{u} = 0 \qquad \nabla \bullet [e \bullet \nabla_s u] = \nabla \bullet [\varepsilon^s \bullet (\nabla \varphi)]$$

Where T is the stress tensor, C_E the elasticity matrix, S the strain tensor, e the piezoelectric coupling matrix, E the electric field vector, D the electrical displacement, ε^s the permittivity matrix, φ the electrical potential, ü is the particle displacement and the particle acceleration.

- **The elasticity matrix, stress matrix and relative permittivity matrix for the XY lithium niobate substrate can be expressed as:**

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & 0 & C_{14} & (C_{11}-C_{12})/2 \end{pmatrix}$$

Elasticity Matrix

$$e = \begin{pmatrix} 0 & 0 & 0 & 0 & e_{15} & -e_{22} \\ -e_{22} & e_{22} & 0 & e_{15} & 0 & 0 \\ e_{31} & e_{31} & e_{33} & 0 & 0 & 0 \end{pmatrix}$$

Stress Matrix

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix}$$

Relative Permittivity Matrix

- **The elasticity matrix for an isotropic material such as gold and PMMA is shown in the following expression. Here, permittivity matrix will have all constants for the principal diagonal elements and the piezoelectric coupling matrix will be zero.**

$$C^E = E/(1+\nu)(1-2\nu) \begin{pmatrix} 1-\nu & \nu & \nu & 0 & 0 & 0 \\ \nu & 1-\nu & \nu & 0 & 0 & 0 \\ \nu & \nu & 1-\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 1-2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-2\nu \end{pmatrix}$$

Elasticity Matrix

Where E is the Young's modulus and v is the Poisson ratio

Micro/Nano Bioengineering Laboratory

Material Constants & Boundary Conditions

	Gold	PMMA
Density	1190 Kg/m^3	19300 Kg/m^3
Poisson Ratio	0.40	0.44
Young's Modulus	3 x 10^{9}Pa	70 x 10^9 Pa

XY Lithium Niobate *

c_{11}	20.3×10^{10} Nm^{-2}
c_{33}	24.5 ×10^{10} Nm^{-2}
c_{44}	6.0×10^{10} Nm^{-2}
c_{12}	5.3×10^{10} Nm^{-2}
c_{13}	7.5×10^{10} Nm^{-2}
c_{14}	0.9×10^{10} Nm^{-2}
e_{15}	3.7 Cm^{-2}
e_{22}	2.5 Cm^{-2}
e_{31}	0.2 Cm^{-2}
e_{33}	1.3 Cm^{-2}
ε_{11}	44
ε_{33}	29
ρ	4600 Kg m^{-3}

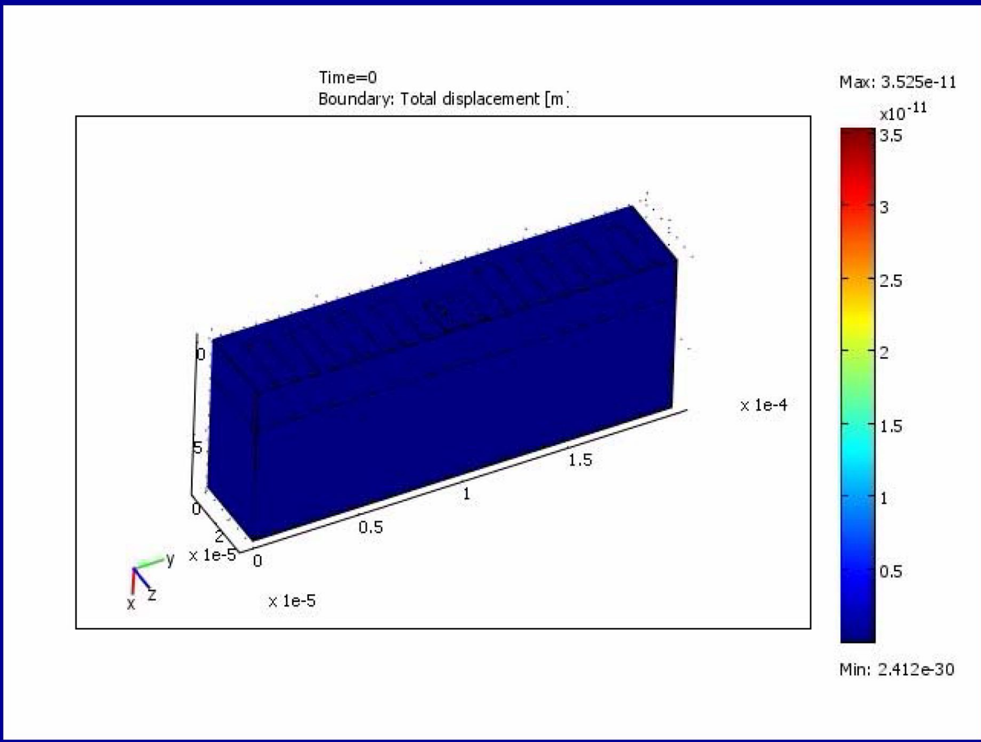
Electrical boundary conditions

Boundary	Electrical Condition
Top boundary of piezoelectric substrate	Zero charge/symmetry
Symmetric plane of piezoelectric substrate	Zero charge/symmetry
All other boundaries of the piezoelectric substrate	Ground
Alternate fingers of generator IDT	Scalar expression for Input wave function
Other fingers of generator IDT	Ground
Alternate fingers of receiver IDT	Zero charge/symmetry
Other fingers of receiver IDT	Ground

*Ref: G. Xu, Direct finite element analysis of frequency response of a Y-Z Lithium Niobate SAW filter, Smart Materials Structures 9 (2000) 973-980.

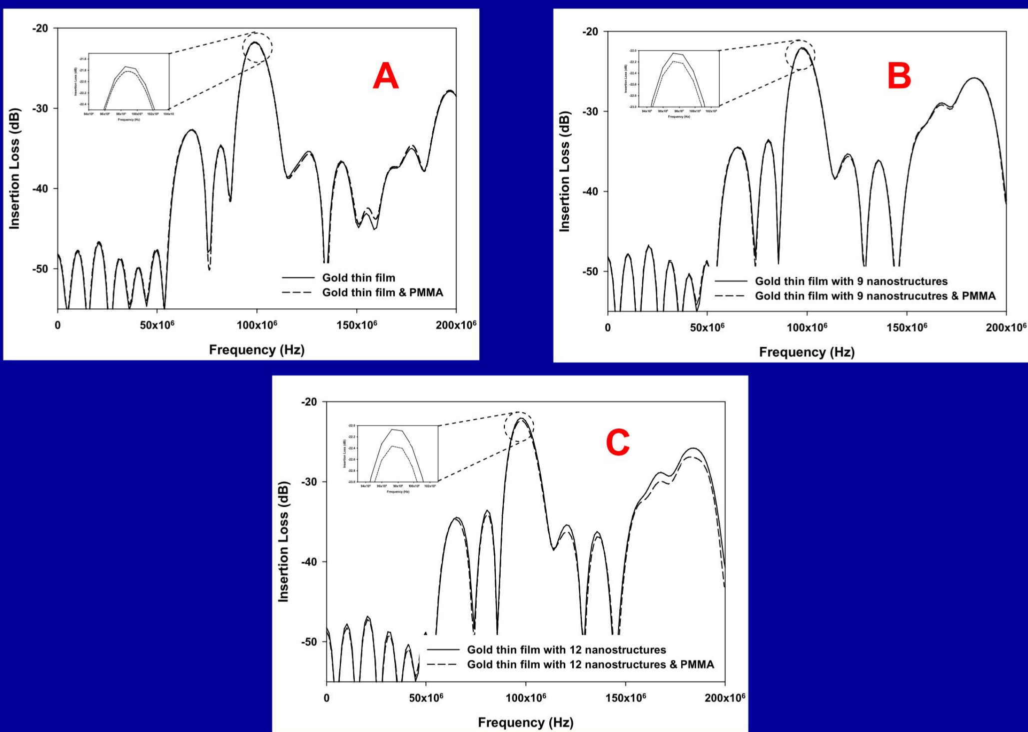
Micro/Nano Bioengineering Laboratory

Results & Discussion



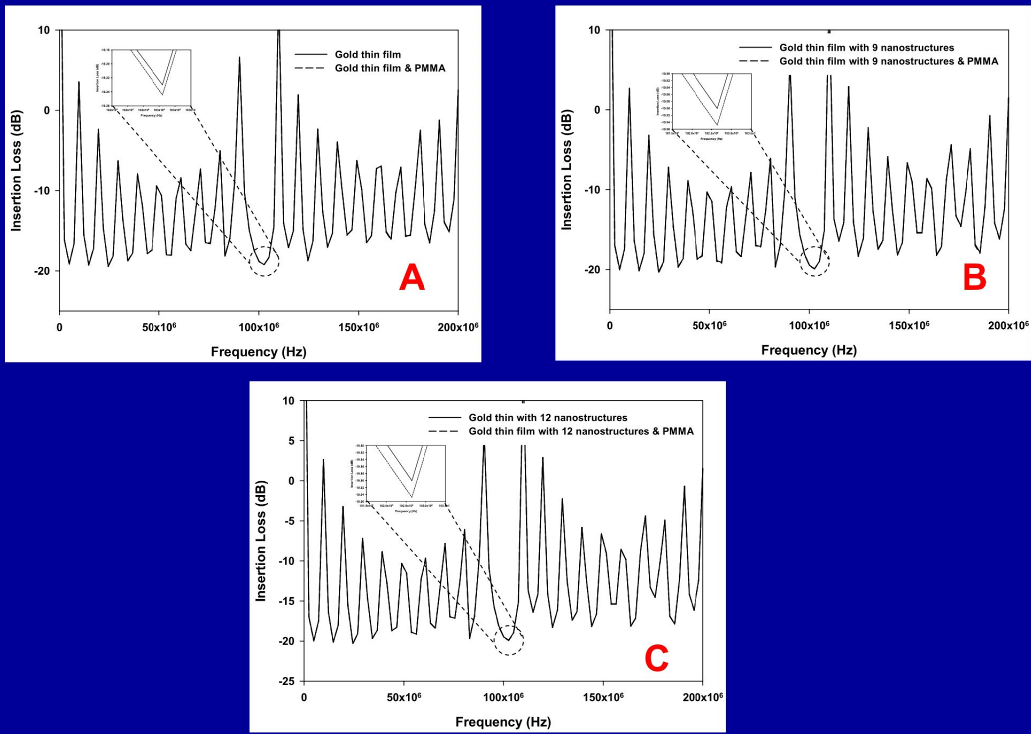
Animated file of total displacement of the 3-D SAW model with a thin film of gold coated on the piezoelectric substrate from 0 to 100nsec.

Results & Discussion



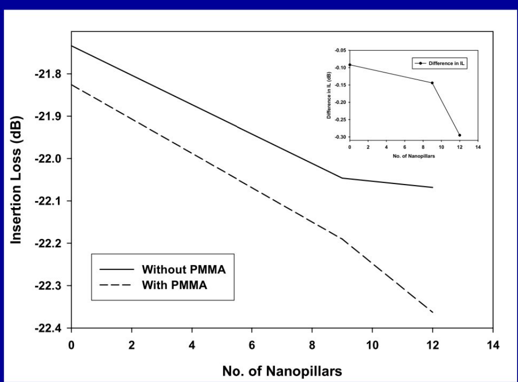
Insertion loss spectra in response to an impulse wave function for a SAW sensor with (A) a gold film as the active surface (B) a gold thin film and 9 nanopillars (C) a gold thin film and 12 nanopillars before and after PMMA adsorption. Inset: Zoom-in view of the peak frequency.

Results & Discussion

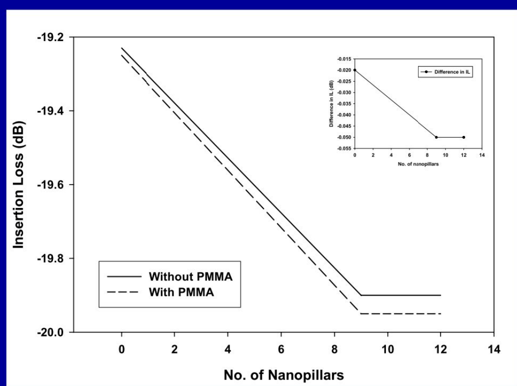


Insertion loss spectra in response to a sinusoidal wave function for a SAW sensor with (A) a gold film as the active surface (B) a gold thin film and 9 nanopillars (C) a gold thin film and 12 nanopillars before and after PMMA adsorption. Inset: Zoom-in view of the peak frequency.

Results & Discussion



Amount of IL in SAW sensors with 0, 9 and 12 nanopillars in response to an impulse wave function before (as a baseline) and after PMMA adsorption. Inset: Difference in IL in reference to the baseline.



Amount of IL in SAW sensors with 0, 9 and 12 nanopillars in response to a sinusoidal wave function before (as a baseline) and after PMMA adsorption. Inset: Difference in IL in reference to the baseline.

Micro/Nano Bioengineering Laboratory