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MIX MATRIX MODELING OF TWO-PORT SURFACE ACOUSTIC WAVE DEVICE FOR PROTEIN CHARACTERIZATION

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ABSTRACT

Presented research describes finite element modeling of Two-Port surface acoustic wave devices used for protein characterization. Typical SAW device converts electrical energy into a mechanical wave on a single crystal substrate. It provides very complex signal processing in a very small volume. It is estimated that approximately 4 billion SAW devices are produced each year. SAW devices are sensitive to temperature, stress, pressure, liquids, viscosity and surface effects, a wide range of sensors are possible. The devices are small, rugged, stable, and capable of high volume low cost production. Research focus is on studying finite element modeling of this devices based on mix matrix methods to characterize conductance, susceptance, viscosity, and other properties of protein samples, like albumin using Two-Port SAW related resonator.

KEYWORDS: Surface Acoustic Wave, Sensors, Characterization, Modeling, Protein.

INTRODUCTION

Previously Dhagat [1] and Kahl [2] et al. used two-port 320 MHz SAW and one port 400–800 MHz SAW resonator respectively. Saluja and Kalonia [3] et al. used 10 MHz using bulk resonators. Two-Port SAW enables precise and controlled measurements as the BSA protein is applied in between the ports. Figure 1 shows the 320 MHz Two-Port SAW resonator filter modified with a channel of width d and depth h cut down the center of the device. Since the electrical and acoustic waves interact linearly, the filter can be decomposed into three sections as shown in fig 2. The computed electrical characteristics of the filter will be independent of the segmentation. The center section is chosen to span the distance d of the channel as shown in fig 2. S1 and S2 correspond to the acoustic waves entering the left and right boundaries respectively. E1 and E2 correspond to the acoustic waves entering the left and right boundaries respectively.

MIX MATRIX FORMALISM

We are going to compute the mixed matrix (derived from a P-matrix formalism) parameters for two-port SAW electro-acoustic cell. Let us first recall the mixed matrix formalism for a cell with two acoustical ports and one electrical port (Fig. 1). The electrical port is characterized by the electrical potential V and the electrical current I. The left (resp. right) acoustical port is characterized by the entering acoustical wave amplitude E_1 (resp. E_2), and the exiting acoustical wave amplitude S_1 (resp. S_2). Let us assume that there are no losses, and that left and right acoustical ports are symmetric. The mixed matrix relates the electrical current and the exiting acoustical wave amplitudes to the entering acoustical wave amplitudes, and the electrical potential.





Figure 1: Mixed Matrix Formalism

2-Port SAW Resonator Filter Design:

Figure 2 shows the 2-port SAW resonator filter modified with a channel of width d and depth h cut down the center of the device. The computed electrical characteristics of the filter will be independent of the segmentation. The center section is chosen to span the distance d of the channel as shown in figure 2. S_1 and S_2 correspond to the acoustic waves exiting the center section from the left and right boundaries respectively. E1 and E2 correspond to the acoustic waves entering the left and right boundaries respectively.

The SAW sensor has a channel width of $d=50.8 \square m$. The center portion of the filter prior to cutting the channel consists of 180 nominally periodic metal strips with a strip period of $p = 4.8486 \square m$. The channel width d can be represented as 10 strip periods plus 2^*dx where $dx = (d-10^*p)/2 = 1.157 \square m$. We can now model the center section of the filter prior to cutting the 50.8 $\square m$ channel as 10 strips plus dx on either side.



Figure 2: 2-port SAW resonator filter with channel of width d and depth h cut down the center of the device.

SAW Resonator Fabrication Process:

Electroacoustic transducers (interdigital transducers) and reflectors can be created using planar electrode structures on piezoelectric substrates. The electrode structure is created by a photolithographic procedure, similar to the procedure used in microelectronics to manufacture integrated circuits as shown in figure 3. Manufacturing begins by carefully polishing and cleaning the piezoelectric substrate. Metal, usually aluminum is then deposited uniformly onto the substrate. The device is spin coated with a photoresist and baked to harden it. It is then exposed to UV light



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through a mask with opaque areas corresponding to the areas to be metalized on the final device. The exposed areas undergo a chemical change that allows them to be removed with a developer. Finally, the remaining photoresist is removed. The pattern of metal remaining on the device is called an interdigital transducer, or IDT. By changing the length, width, position, and thickness of the IDT, the performance of the sensor can be maximized.



Figure 3: 2-port SAW resonator device fabrication process.

Mix-Matrix Analysis:

A complete filter analysis can be made using the three matrix equations given in figure 4. Since the electrical and acoustic waves interact linearly, the filter can be decomposed into three sections as shown in figure 4. Due to symmetry the MIX matrix of both outer sections is identical. It is assumed that no acoustic waves enter the structure from the ends, so it is only necessary to include one acoustic port for both outer sections. The center matrix is called a diffraction matrix since there are only acoustic ports.



Figure 4: MIX matrix equations describing each section of the 2-port SAW resonator filter.

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The matrices form six algebraic equations with eight variables: V_1 , V_2 , I_1 , I_2 , E_1 , E_2 , S_1 , and S_2 . By eliminating the four acoustic variables we can derive the 2-port admittance matrix for the structure.

$$\begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} Y_{11} & Y_{12} \\ -Y_{21} & Y_{22} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}$$
(1)

A nominal analysis of the outer section and center section has been made using Phonon proprietary analysis software. The results are tabulated vs frequency for the following matrix elements:

Yt, Ct, Rt, R_1 , T, and R_2

The admittance matrix elements in equation 1 for the filter can be written in terms of the above 6 elements vs frequency. The resulting admittance matrix will correspond to the unmodified filter and will correlate well with a measured filter.

The sensor with liquid in the cut channel can be modelled by modifying R_1 , T, and R_2 in the diffraction matrix of the center section vs frequency (equation 2).

$$\binom{S_1}{S_2} = \binom{R_1 \ T}{T \ R_2} \binom{E_1}{E_2} \quad (2)$$

The elements R_1 , T, and R_2 are the deterministic paramters of the sensor.

RESULTS AND DISCUSSION

The Mix matrix numerical model has been used to compute the admittance matrix for the 2-Port SAW transducer. A typical analysis result for Y_{12} using this model is shown below at different temperatures in presence of DI water.



Fig. 5a. Simulated Amplitude and Phase change in presence of DI Water at different temperatures

Fig. 5b. Simulated Amplitude and Phase change in presence of DI Water at different temperatures with 2.5pF I/O Coupling





Fig. 6. Simulated Amplitude and Phase change in presence of DI Water at 30°C with 2.5pF I/O Coupling

Derivations:

$$\begin{pmatrix} I_1 \\ E_1 \end{pmatrix} = \begin{pmatrix} Y_t & C_t \\ -C_t & R_t \end{pmatrix} \begin{pmatrix} V_1 \\ S_1 \end{pmatrix} \quad (1a)$$

$$\begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \begin{pmatrix} R_1 & T \\ T & R_2 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} \quad (2b)$$

$$\begin{pmatrix} I_2 \\ E_2 \end{pmatrix} = \begin{pmatrix} Y_t & C_t \\ -C_t & R_t \end{pmatrix} \begin{pmatrix} V_2 \\ S_2 \end{pmatrix} \quad (3b)$$

In the equation set 1-3 there are two independent variables (V_1 , V_2), four intermediate variables, (S_1 , E_1 , S_2 , E_2) and two dependent variables (I_1 , I_2) which we have to solve for. Eliminating the four intermediate variables the two port admittance matrix for the device can be obtained.

$$\begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} Y_{11} & Y_{12} \\ -Y_{21} & Y_{22} \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}$$

The mechanics of the derivation are as follows. Equations 2(a,b) relate S1 and S2 in terms of E1 and E2

$$\begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \begin{pmatrix} R_1 & T \\ T & R_2 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} \begin{pmatrix} 2a \\ (2b) \end{pmatrix}$$

Equations 2a implied $S_1 = R_1E_1 + TE_2$ Equations 2b implied $S_2 = TE_1 + R_2E_2$

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Replace S₁ and S₂ in equations 1b and 3b with the equations 2a and 2b respectively.

$$\begin{pmatrix} I_1 \\ E_1 \end{pmatrix} = \begin{pmatrix} Y_t & C_t \\ -C_t & R_t \end{pmatrix} \begin{pmatrix} V_1 \\ S_1 \end{pmatrix} \quad (1a) \qquad \qquad \begin{pmatrix} I_2 \\ E_2 \end{pmatrix} = \begin{pmatrix} Y_t & C_t \\ -C_t & R_t \end{pmatrix} \begin{pmatrix} V_2 \\ S_2 \end{pmatrix} \quad (3a)$$

The modified 1b and 3b are then combined to form a new matrix equation defined by equations 4a and 4b below. Then, after some matrix manipulation we obtain the following matrix equation.

$$\begin{pmatrix} \mathbf{1} - R_t R_1 & -R_t T \\ -R_t T & \mathbf{1} - R_t R_2 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = \begin{pmatrix} -C_t & \mathbf{0} \\ \mathbf{0} & -C_t \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \begin{pmatrix} 4a \\ 4b \end{pmatrix}$$

Solve equation 4 for E1 and E2

$$\begin{pmatrix} E_1 \\ E_2 \end{pmatrix} = \begin{pmatrix} \mathbf{1} - R_t R_1 & -R_t T \\ -R_t T & \mathbf{1} - R_t R_2 \end{pmatrix}^{-1} \begin{pmatrix} -C_t & \mathbf{0} \\ \mathbf{0} & -C_t \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \begin{pmatrix} \mathbf{5}a \end{pmatrix}$$
(5b)

Combine equation 2 and 5

$$\binom{S_1}{S_2} = \binom{R_1 T}{T R_2} \binom{1 - R_t R_1 - R_t T}{-R_t T 1 - R_t R_2}^{-1} \binom{-C_t 0}{0 - C_t} \binom{V_1}{V_2} \binom{(6a)}{(6b)}$$

From equation 6 we can define a new matrix called Q-Matrix

$$\begin{pmatrix} Q_{11} Q_{12} \\ Q_{21} Q_{22} \end{pmatrix} = \begin{pmatrix} R_1 T \\ T R_2 \end{pmatrix} \begin{pmatrix} 1 - R_t R_1 & -R_t T \\ -R_t T & 1 - R_t R_2 \end{pmatrix}^{-1} \begin{pmatrix} -C_t & 0 \\ 0 & -C_t \end{pmatrix}$$
(7)

Then equation 6 can be modified as

$$\binom{S_1}{S_2} = \binom{Q_{11} Q_{12}}{Q_{21} Q_{22}} \binom{V_1}{V_2} \binom{(8a)}{(8b)}$$

We can rewrite equation 1a as

$$I_1 = Y_t V_1 + C_t (Q_{11} V_1 + Q_{12} V_2) = (Y_t + C_t Q_{11}) V_1 + C_t Q_{12} V_2 \quad (9)$$

Equation 3a can be re-written as

$$I_2 = Y_t V_2 + C_t (Q_{21} V_1 + Q_{22} V_2) = C_t Q_{21} V_1 + (Y_t + C_t Q_{22}) V_2$$
(10)

From euqations 9 and 10 we can say

$$\begin{pmatrix} Y_{11} Y_{12} \\ Y_{21} Y_{22} \end{pmatrix} = \begin{pmatrix} Y_t + C_t Q_{11} & C_t Q_{12} \\ C_t Q_{21} & Y_t + C_t Q_{22} \end{pmatrix} (11)$$

Where the Q-Matrix is defined by Equation 7 as shown below

$$\begin{pmatrix} Q_{11} Q_{12} \\ Q_{21} Q_{22} \end{pmatrix} = \begin{pmatrix} R_1 & T \\ T & R_2 \end{pmatrix} \begin{pmatrix} 1 - R_t R_1 & -R_t T \\ -R_t T & 1 - R_t R_2 \end{pmatrix}^{-1} \begin{pmatrix} -C_t & 0 \\ 0 & -C_t \end{pmatrix}$$
(7)

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Tables:

| Elastic Matrix In Stiffness Form (x10 ¹⁰ Pa) | | Piezoelectric Matrix at Constant Strain (C/m2) | | Permittivity Matrix at Constant Strain (x10 ⁻¹¹ F/m) | |
|--|--------|---|--------|--|-------|
| C ₁₁ | 8.679 | e ₁₁ | 0.1711 | ε ₁₁ | 3.992 |
| C ₁₂ | 0.679 | e ₁₄ | 0.4060 | ε ₃₃ | 4.104 |
| C ₁₃ | 1.200 | | | | |
| C ₁₄ | 1.811 | | | | |
| C ₃₃ | 10.579 | | | | |
| C ₄₄ | 5.821 | | | | |
| C ₆₆ | 4.000 | | | | |

Table 1. Material Constants of Quartz Wafer

CONCLUSION

We have successfully demonstrated simulated results of a SAW sensor to detect characteristics of a Protein using Mix Matrix Finite Element Analysis. Sensors show a linear relation of admittance data with respect to BSA. A MIX matrix based computational model accurately predicts device behavior of the SAW and fluid interactions. Rigorous analysis of the data to show conductance, susceptance, admittance, resistance, and impedance will establish this research as a comparable study in the SAW sensors field.

A coupled FEM/BIE numerical model has been used to compute the harmonic admittance of aperiodic multielectrode transducers. The MIX matrix elements can be extracted from the results. These calculations are used to improve the models and accuracy of the analysis software. The model has been successfully used to improve the analysis of SAW devices incorporating modified HanmaHunsinger cells and unbalanced split-finger triplet cells.

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