Modelling and Simulation using Finite Element Method of Surface Acoustic Wave Biosensor for Gas Detection Application

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Abstract. A surface acoustic wave (SAW) sensor detects changes in physical properties such as mass and density on its surface. Compared to other types of sensors, SAW sensor have a good stability, high selectivity and sensitivity, fast response, and low-cost. On the other hand, to design and optimize a SAW biosensor requires a long process including time and cost using conventional methods. Therefore, numerical simulation and computational modelling are useful and efficiently conduct analysis for the SAW biosensor. In this paper, a numerical simulation technique is used to analyse the SAW device sensitivity for the application of gas detection. The SAW biosensor can detect very small mass loading by changing its sensor resonance frequency. The two-dimensional (2D) device model is based on a two-port SAW resonator with a gas sensing layer. We made two design of SAW biosensor device with frequency of 872 MHz and 1.74 GHz. A gas with vary concentration from 1 to 100 ppm were used to determine the change of the device resonance frequency. As a result, the high frequency (1.74 GHz) device, shows that the resonance frequency is shifted larger than to the low frequency (872 MHz) device. In addition, the high frequency device offers five times more sensitivity than the low frequency device. By changing the sensor design, the sensor characteristics such as sensitivity can be altered to meet certain sensing requirements. Numerical simulation provides advantages for sensor optimization and useful for nearly representing the real condition.

1. Introduction

Biosensors are a device that convert biological information to electronic, optical, magnetic, or acoustic signals suitable for quantitative measurement. A biosensor is typically comprising of a biochemical recognition system and a transducer that converts the biochemical response to a measurable output signal. Furthermore, it can be used to quantify biological or chemical processes by generating signals proportional to the concentration of an analyte present in the reaction. As an example, a surface acoustic wave (SAW) sensor uses interdigit electrodes (IDTs) to convert electric signals to acoustic waves, which can be altered by sensing event. SAW device have been used as sensors due to their sensitivity toward surface perturbations. These sensors work by sensing an acoustic wave travelling through or along the surface of a piezoelectric substance and sometimes it is identified as transverse wave. Due to their exceptional sensitivity and advantages, acoustic wave sensors have attracted a lot of attention recently [1]. Additionally, acoustic wave technologies offer numbers of benefits, including ease of use, high sensitivity, compact size, rapid reaction, and low cost. Furthermore, acoustic wave sensors not only can...
detect changes in mass and density, but also in viscosity, elastic modulus, conductivity, and dielectric characteristics.

Biosensors are employed in a range of applications, including illness monitoring, drug discovery, and the detection of contaminants, pathogens, and disease markers in physiological fluids (blood, urine, saliva, sweat). Sensor based on surface acoustic waves (SAW) have concentrated acoustic energy on the surface, which increases their sensitivity to surface disturbance. As a result, SAW sensor has a great sensitivity for detecting extremely small charges on the surface. In addition, SAW sensors are well suited for biosensor tasks due to their ability to detect surface changes such as mass loading effects. While, the surface acoustic wave biosensor is critical for biological clinical detection, its sensitivity and specificity can yet be improved. For example, the structure of the surface acoustic wave biosensor, including the dimensions, materials, and forms of the interdigital transducers, influenced the sensor's sensitivity [2]. Additionally, the amplitude-frequency response of the sensor has a significant effect on its performance, especially its sensitivity.

This paper investigated the relationship of surface acoustic wave (SAW) device sensitivity for a gas detection application. The simulation is based on a two-dimensional (2D) model that represents a partial area of the sensor. The dimension of the device IDT is adjusted to alter the device's frequency response. We model a low and high frequency SAW biosensor with estimated 872 MHz and 1.7 GHz accordingly. For high frequency device, the sensitivity increased compared to low frequency device, making it potentially useful for mass sensing such as gas detection application.

2. Mathematical model of SAW device
A biosensitive layer is applied to the SAW device surface, which is then utilized to convert tiny quantities of biological information into electrical signals that the equipment can detect through the two interdigital transducers (IDTs). Figure 1 shows the schematic design for the SAW biosensor described in this paper.

The SAW biosensor devices are made of piezoelectric materials, which are utilized for signal conversion due to their positive and negative piezoelectric properties. When a SAW propagates through piezoelectric materials, electromagnetic waves are produced as a result of the induced charge. Thus, it is usually necessary to consider both Maxwell and motion equations in conjunction with the piezoelectric equation when describing SAW propagation on piezoelectric materials [3][4]. The equation of motion of a particle in an elastic medium is defined as

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial^2 T_{ij}}{\partial x_j} \quad (i, j = 1, 2, 3)$$

(1)

where $u_i$ indicates the particle's displacement in the $x_i$ direction, $\rho$ indicates the particle's bulk density, and $t$ indicates the time. The relationship between stress, $T_{ij}$, strain, $S_k$, and electric field strength, $E_k$, in a medium can be expressed as follows utilizing the piezoelectric equation.

$$T_{ij} = c_{ijkl} E_k S_l - e_{ijk} E_k$$

(2)

Where $c_{ijkl}$ indicates the constant of elastic stiffness in a constant electric field and $e_{ijk}$ indicates the piezoelectric constant. Since electromagnetic waves have a velocity of several orders of magnitude greater than the SAW acoustic waves, the electromagnetic field related to the SAW device can be described by an electrostatic field, and $E_k$ is expressed as a gradient of the potential function.

$$E_k = -\frac{\partial \phi}{\partial x_k} \quad (k = 1, 2, 3)$$

(3)

Additionally, the following relationship exists between strain and particle displacement in the blank holder material by
\[ S_{kl} = \frac{\partial u_k}{\partial x_l} \quad (k, l = 1, 2, 3) \]  

(4)

From equations (1), (2), (3), and (4), it is possible to obtain that,

\[ P \frac{\partial^2 u}{\partial t^2} = c_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} + e_{ijk} \frac{\partial^2 \phi}{\partial x_k \partial x_j} \]  

(5)

Due to the insulating nature of the medium and the absence of free charge, the divergence of the electrical displacement vector, \( D \) must equal zero, that is

\[ \nabla \cdot D = \frac{\partial D_j}{\partial x_j} = 0 \quad (j = 1, 2, 3) \]  

(6)

The piezoelectric equation of the medium may be described as

\[ D_j = e_{jk} S_{kl} + \varepsilon_{jk} E_k \]  

(7)

where \( \varepsilon \) is the dielectric constant of the material. Combining equations (3), (4), (6), and (7) gives the coupling equation.

\[ e_{jkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} - \varepsilon_{jlk} \frac{\partial^2 \phi}{\partial x_j \partial x_k} = 0 \]  

(8)

The coupling equations in piezoelectric materials are represented by equations (5) and (8). The elastic wave characteristics of piezoelectric materials is explained by the equations.

### 3. SAW biosensor model

The major components in SAW biosensor are the IDT and the type of substrate used (Figure 1(a)). The input IDT convert the input signal which is an alternating current, and the substrate converts this electrical signal into the acoustic signal by the principle of piezoelectric effect. This effect which is the deformation of the piezoelectric substrate surface that propagates along the surface until it reached the other end of the output IDT. This output IDT then convert the acoustic signal that propagates back to the electrical signal. Figure 2(a) shows the 2D model of SAW biosensor.

In the SAW biosensor device, piezoelectric substrate materials are used. The properties of this materials greatly influenced the performance of the device. Many researchers developed SAW devices using materials such LiNbO\textsubscript{3}, LiTaO\textsubscript{3}, ST-X Quartz, AlN, GaAs, ZnO, La\textsubscript{3}Ga\textsubscript{5}SiO\textsubscript{14}. On the other hand, the IDT structure and dimension is also important for the sensing performance. In this simulation model, the IDT fork-finger is identified as \( a \), with spacing, \( b \) and the sound aperture, \( w \) as shows in the Figure 1(c). A piezoelectric substrate is based on LiNbO\textsubscript{3} (YZ-cut) which suitable for high frequencies application and high temperature coefficient values. The aluminum material is selected for the IDT electrode. Aluminum have very low density and acoustic impedance, which reduced the effect to the resonance frequency and, having very high conductivity and ease of fabrication process. For the gas sensing application, dichloromethane (CH\textsubscript{2}Cl\textsubscript{2}) was selected. In addition, gas sensing layer should have a good selectivity to detect gas, therefore the sensing layer is model based on composites polyisobutylene and carbon nanotubes.

The finite element simulation for the 2D SAW biosensor model were performed using COMSOL (COMSOL, USA) software. 2D model was choose due to high requirements such as computer processing and memory capability including time factors for high resolution three-dimensional (3D) model data. Moreover, 2D model reduce the computational cost, although it is not a finalize result for designing a SAW biosensor, however, it provides enough analysis and estimation for studying the sensor
frequency response characteristics typically. The detail of the model boundary conditions shows in Table 1.

**Figure 1.** SAW device. a) SAW biosensor with two-port. (b) Periodic boundary condition for 2D model simulation. (c) IDT dimension

| Table 1. Boundary parameters |
|-----------------------------|
| **Design Type** | **Boundary** | **Value** | **Unit** |
| Design 1 (D1) | IDT finger width (a) | 1 | µm |
| | IDT spacing (width) (b) | 2 | µm |
| | Estimated resonance frequency | 872 | MHz |
| Design 2 (D2) | IDT finger width (a) | 0.5 | µm |
| | IDT spacing (width) (b) | 1 | µm |
| | Acoustic wave velocity | 3488 | m/s |
| | Estimated resonance frequency | 1.744 | GHz |
| | Substrate (LiNO3) | YZ-Cut (12x20) | µm |
| | Acoustic wave velocity | 3488 | m/s |
| | Voltage Potential | 1 | V |
| | Gas concentration | 1-100 | ppm |
4. SAW biosensor frequency response analysis

In this work, we investigated the frequency response of the SAW biosensor. The device resonance frequencies should be slightly changed as the mass of the sensing layer increases. For example, when the sensing layer absorbs the selective gas, the mass layer expands, changing the frequency response. A slight change in mass causes the resonance to change at very high frequencies by

\[ \Delta f = -\frac{k \Delta m f_0^2}{A} \]  

(9)

where \( k \), represents the spring or material constant, \( m \) represents the mass loaded, \( f_0 \) represents the resonance frequency and \( A \), represents the area. This demonstrates that altering the resonance frequency results in an increase in the system's shift because of mass loading. Thus, the SAW device's sensitivity will be determined by comparing the resonance frequency changes between the two designs. There are two conditions applied: with and without adsorbed gas.

5. Result and discussion

The devices resonance frequency and the symmetrically mode are analyzed. The resonance frequency estimated as shows in Table 1. On the other hand, the resonance frequency obtained from the simulation resulted a close to the estimation values. Figure 2 shows the resonance frequencies eigenmode for D1 and D2 sensors.

![Figure 2. SAW device eigenmode analysis. (a) 849 MHz (b) 855 MHz (c) 1.278 GHz (d) 1.693 GHz (displacement magnitude scale in µm)](image)

For the D1 device, the frequency responses are 849 MHz and 855 MHz, while for the D2 device, are 1.2 GHz and 1.7 GHz. These frequency responses include anti-resonance frequency which is the minimum amplitude occur at D1 and D2 devices where the affected frequencies are 841 MHz and 1.2 GHz respectively. On the other hand, the devices frequency response values were determined based on the eigenmode analysis which the displacement of deformed shape (standing wave) on the substrate top surface to the surface. In addition, the displacement fades exponentially to the bottom.
Figure 3 shows an example of a device effect (inverse piezoelectric effect) when a voltage is applied. At a frequency of 855 MHz for the D1 device, the maximum deformation values are about $3.5 \times 10^{-5}$ μm and the 1.7 GHz frequency for D2 device is about $19 \times 10^{-4}$ μm. The device surface deformation is related to the mechanical stress relationship in stress-charge form is defined as

\[ S = S_E T + d^T E \]  

(10)

\[ D = d T + \varepsilon_0 \varepsilon_r E \]  

(11)

where $S$ is the strain, $D$ is the electric displacement field, $T$ is the stress, and $E$ is the electric field. Therefore, at high frequency D2 device (1.7 GHz), the displacement is higher compared to the low frequency D1 device (855 MHz).

Additionally, as explained in previous topic, the frequency shifted because the sensing layer mass loading changed as shown in equation (9). Therefore, the presence of gas changes in the surface wave velocity due to the are proportional to changes in the oscillation frequency.

The amplitude displacement of resonance frequency for D2 devices higher than the D1 devices. These significant different of shifted frequency for D2 devices as instance, will make the sensor detection circuitry be able to detect a very small gas concentration and increase the sensor signal-to-noise ratio value, which improves the device's sensitivity. As shows in Table 2, the differences of frequency response for both designs during condition zero (0 ppm) and maximum (100 ppm) gas concentration. The D2 1.69 GHz SAW device offers five times sensitivity (sensor response) compared to the 855 MHz one in mass elastic loading. Figure 3 shows the frequency response of D1 and D2 with gas concentrations varies from 1 to 100 ppm. The frequency decreased as concentration increasing due to change of sensing layer density.

Table 2. Frequency response at zero (0 ppm) and maximum (100 ppm) concentration

|                  | At condition zero | At condition max. | $\Delta F$ | $\Delta$ Avg. magnitude displacement (μm) | Sensor response (Hz ppm$^{-1}$) |
|------------------|-------------------|-------------------|------------|------------------------------------------|---------------------------------|
| **Frequency (MHz)** |                   |                   |            |                                          |                                 |
| **D1**           | 849.025247        | 849.025078        | 0.000169   | $3.543 \times 10^{-5}$                   | 2                               |
|                  | 855.483793        | 855.483570        | 0.000223   | $5.708 \times 10^{-5}$                   | 2                               |
| **D2**           | 1278.916436       | 1278.915959       | 0.000477   | $4.319 \times 10^{-4}$                   | 5                               |
|                  | 1693.595738       | 1693.559471       | 0.036270   | $4.809 \times 10^{-4}$                   | 10                              |

![Figure 3. SAW frequency response](image-url)
6. Conclusion
This paper presents the 2D model numerical simulation studies for SAW Biosensor device. The simulation studies are useful for further analysis and design of SAW device. 2D model with periodic boundary structure may reduce the computational cost, however the behaviour of the periodic structure may not present the whole SAW device. Further study using numerical simulation in 3D model is preferable to reduce the spurious modes and development of new-type SAW devices configured with complex structures and applications.

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