SURFACE ACOUSTIC WAVE GAS SENSOR

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Abstract – Surface acoustic wave (SAW) resonators represent some of the most prominent acoustic devices for chemical sensing applications. As their frequency ranges from several hundred MHz to GHz, therefore they can record remarkably diminutive frequency shifts resulting from exceptionally small mass loadings. Their miniaturized design, high thermal stability and possibility of wireless integration make these devices highly competitive. Owing to these special characteristics, they are widely accepted as smart transducers that can be combined with a variety of recognition layers based on host-guest interactions, metal oxide coatings, carbon nanotubes, graphene sheets, functional polymers and biological receptors. As a result of this, there is a broad spectrum of SAW sensors, i.e., having sensing applications ranging from small gas molecules to large bio-analytes or even whole cell structures. This review shall cover from the fundamentals to modern design developments in SAW devices with respect to interfacial receptor coatings for exemplary sensor applications. The related problems and their possible solutions shall also be covered, with a focus on emerging trends and future opportunities for making SAW as established sensing technology.

I. INTRODUCTION

Since the first reported use of a surface acoustic wave (SAW) delay-line (DL) oscillator as a mean to characterize delay-time variation with temperature for $LiNbO_3$, there has been considerable interest evidenced in both SAW delay-line and resonator-based oscillators, Much of this attention has focused on application involving radar, avionic, and satellite communication systems.

Although there are many reasons behind this high level of interest, the five principal motivating factors are as follows.

1) Fundamental frequency oscillator operation spanning the range of 100 MHz to 2000 MHz This wide range of operation affords reduced cost, size, and power consumption when compared to alternative techniques, such as frequency multiplication/filtering/amplification, using a much lower frequency bulk-acoustic-wave (BAW) oscillator.

2) SAW delay-line or resonator-based oscillators offer frequency stability approaching that of quartz-crystal BAW oscillators. The choice between delay lines and resonators offers the designer considerable flexibility in selecting modulation range and phase noise level.

3) The relative ease of SAW device fabrication and compatibility with most standard microelectronic processing techniques.

4) The inherent ruggedness of the device, since its frequency is established by the periodicity of the inter digital transducer and/or reflector patterns on the surface of the substrate, and not the physical dimensions of the device.

5) Finally, the considerable effort that has gone into the development of BAW oscillators over the last 60 years, especially improvements in quartz substrate material, substrate cleaning and processing technology, and device packaging techniques, has leveraged the effort to develop precision SAW oscillator.

Fig. 1 shows a simple block diagram for a generalized SAW stabilized feedback-loop oscillator design. Although individual oscillators will differ in their specifics, they all share the following common features:

1) One or more loop amplifiers (G_1, G_2) of enough gain to overcome total feedback loop losses.
2) Some means for gain limiting (compression) within the feedback loop to ensures table oscillation (in many instances this gain-limiting action may occur in the second stage or high-level feedback-loop amplifier).
3) Provisions for gain and phase adjustment within the feedback loop to establish approximately *3dB (2-4dB)* of excess small-signal gain (nominally *3dB* of gain compression

when equilibrium is reached) and $27\pi N$ net phase shift, where N is an integer.

4) Feedback-loop signal sampling, which may be either capacitive, resistive, etc.

5) A buffer amplifier (G_3) to isolate the feedback loop from load variations. The need for electronic phase shift in the feedback loop to provide frequency modulation and a low-pass filter at the oscillator's output to suppress spurious harmonic signals may or may not be necessary depending upon specific performance requirements.

The SAW device may be either a two-port delay line or resonator, as illustrated in Figs. 2(a) and 2(b). respectively, or a one-port resonator as shown in Fig. 2(c). When used in a "pseudo two-port" configuration, as shown in Fig. 3(b), the transmission characteristic of the one-port resonator is dominated by the static transducer capacitance C_0’. This is illustrated in Fig. 4(a). A parallel inductor may be used to tune-out C_0’ and the result is shown in Fig. 4(b). The response near the acoustic resonance is now very clean, but the low insertion loss at both high and low frequencies presents problems. Even when used in a conventional impedance-controlled (negative resistance) oscillator such that as circuit, in Fig. 5, these problems persist, along with a marked sensitivity to circuit

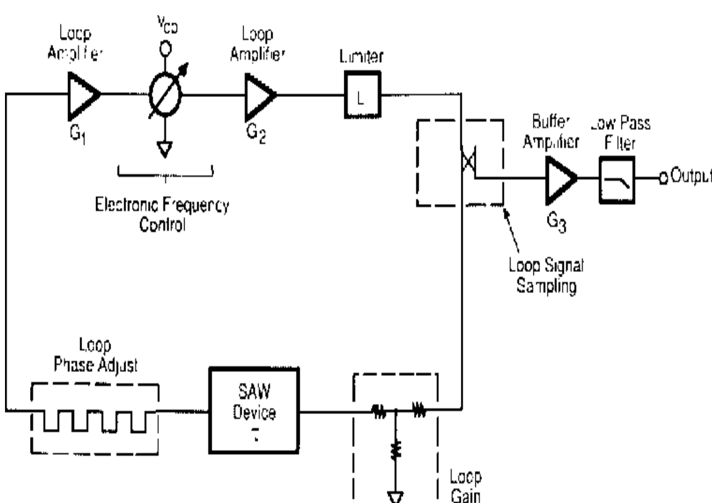


Fig. 1. Block Diagram of feedback loop oscillator

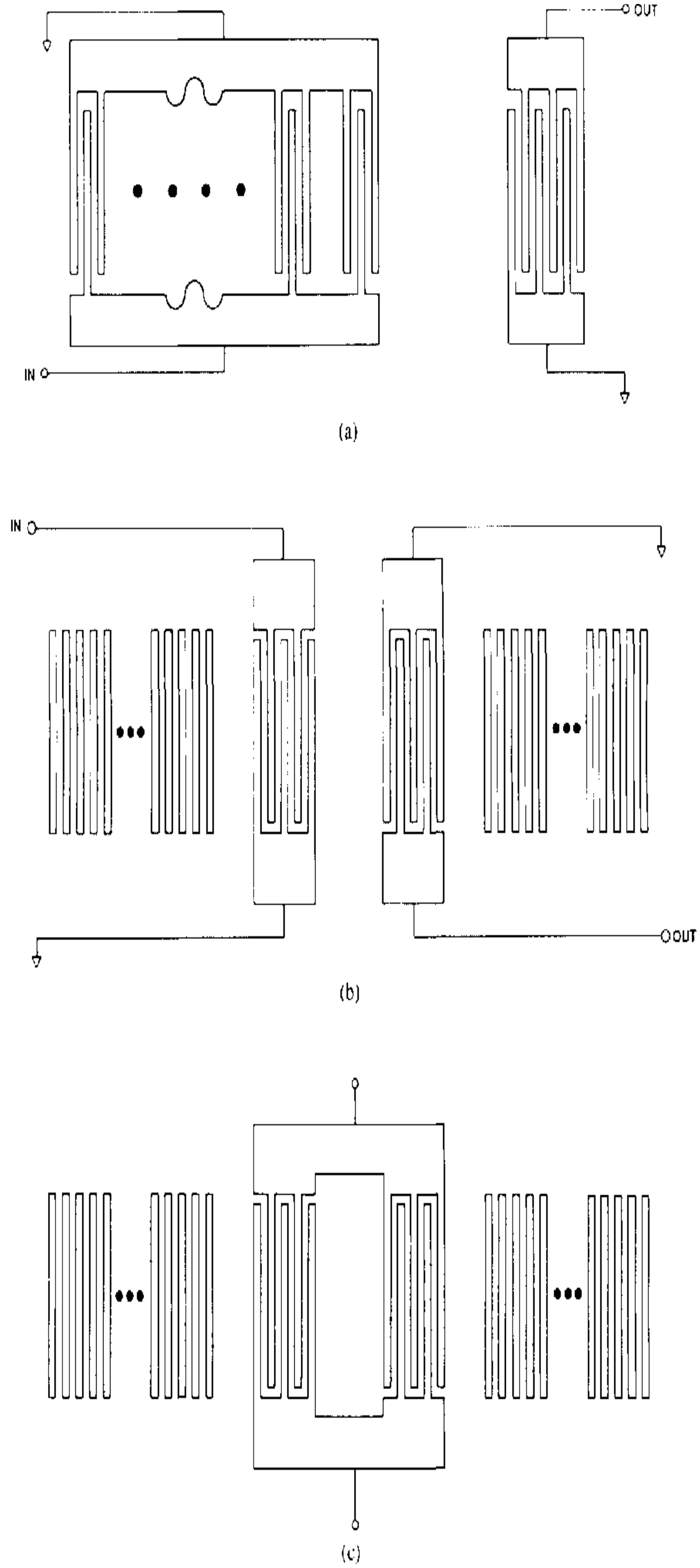


Fig. 2. Two-port and one-port SAW devices, (a) Two-port delay line. (b) Two-port resonator. (c) One-port resonator

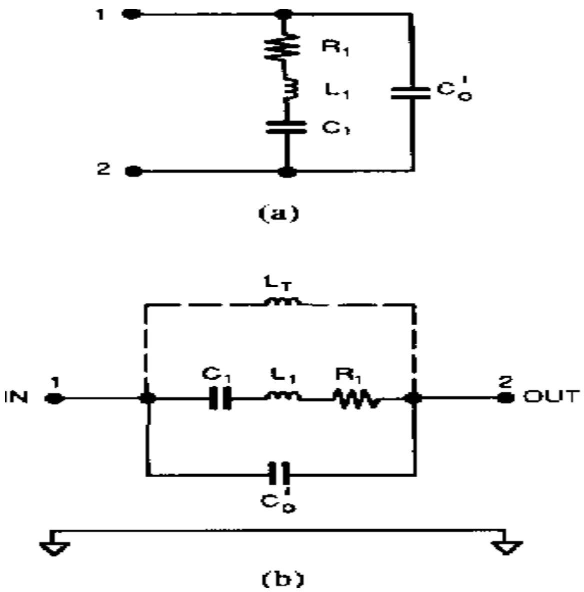


Fig. 3. One-port SAW resonator. (a) Electrical equivalent circuit. (b) “Pseudo two-port” electrical connection for one-port resonator, including external inductor L, to tune out static transducer capacitance C0’

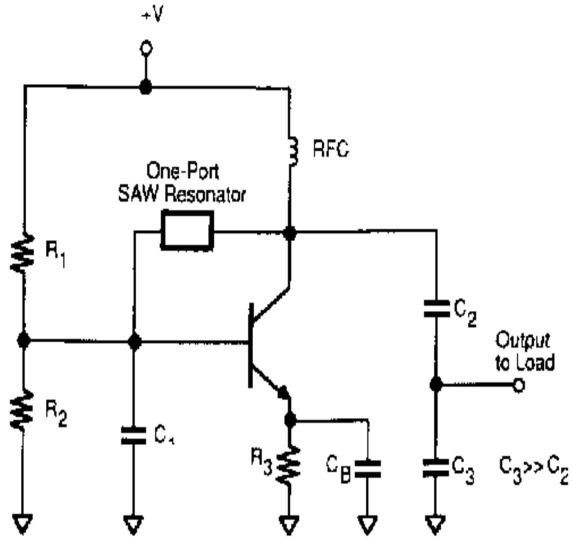


Fig. 5. Schematic diagram of Pierce oscillator circuit, including one-port SAW resonator

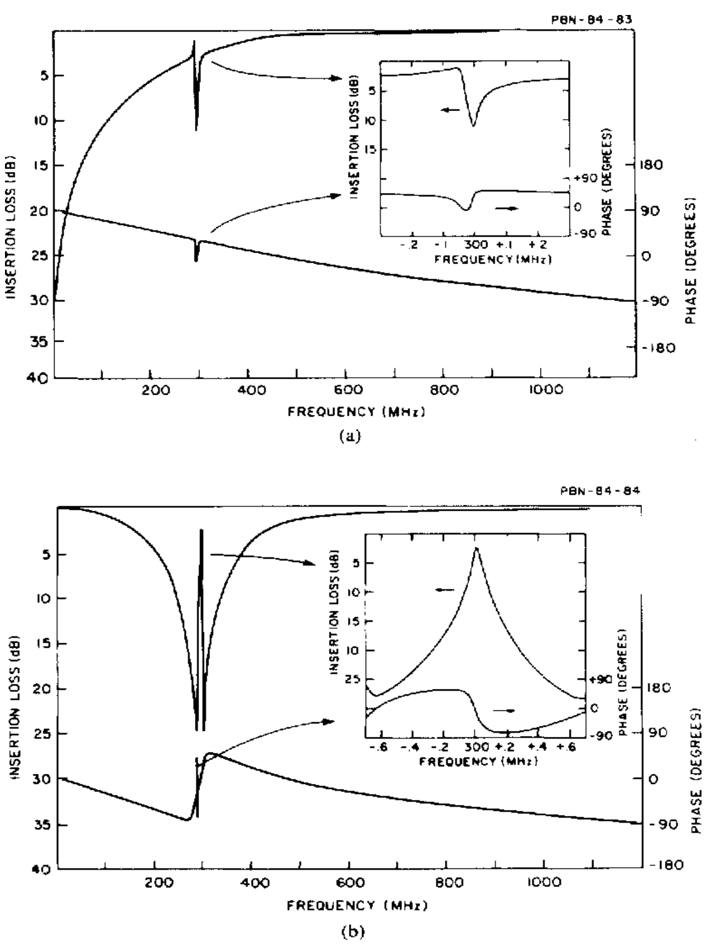


Fig. 4. Insertion loss and phase responses for “pseudo two-port” resonator connection shown in Fig. 3(b). (a)Without inductor L_T, (b) With inductor L_T

II. WORKING PRINCIPLE

SAW sensors are indirect probes of various physical and chemical quantities. The presence of an entity in the propagation path of the surface waves causes a change in the phase velocity and amplitude of the waves. For chemical sensing, these changes are induced by variation in properties (to be discussed below) of a coated sensing layer on the piezoelectric transducer upon exposure to target analytes (Fig. 6). By detecting these changes at the output IDT via the converted electric signal, one can obtain quantitative information about the analyte.

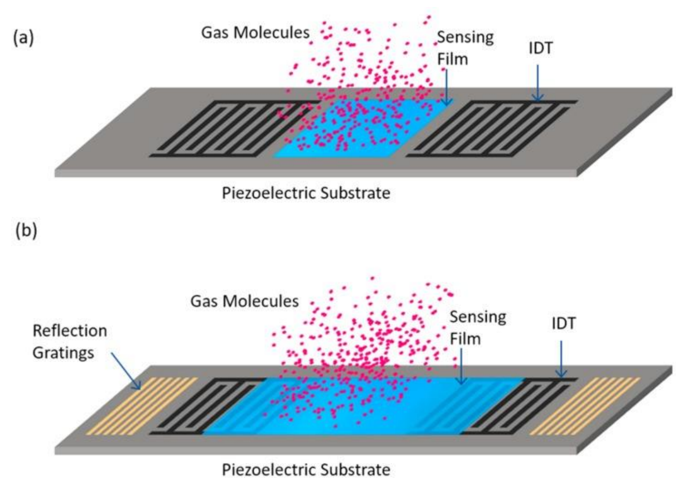


Fig. 6. Schematics of SAW chemical sensors: a two-port delay line (a) and a resonator (b) with sensing overlayers and target analyte vapours.

To excite the SAWs and detect the changes, two types of device configurations, namely the delay lines and the resonators (Fig. 6 (a) & (b) respectively), are commonly used. A typical 'delay line' SAW sensor consists of two IDTs deposited on a piezoelectric substrate at a certain separation, one for input and one for output of the electric signal. The region between the IDTs is coated with a recognition layer for interaction with foreign chemical vapors or gases. This region creates a delay in time between the input and output signals based on its length and the SAW velocity. Fig. 6 a show a two-port delay line configuration of the SAW devices. It is also possible to use a single IDT for both purposes, the excitation and detection, by providing a reflector (usually another IDT). This is the one port or reflective delay line configuration. A delay line requires enough impedance matching for a tolerable insertion attenuation. In addition, oscillator circuit design becomes complicated in this configuration as it offers relatively large phase changes (~2π) in its passband. However, this configuration is simple and practical for sensing applications.

The second configuration type of the devices is the 'resonator' that consists of two IDTs for emission and detection of the acoustic waves and grating reflectors are placed outside of each IDT so that a resonating cavity is formed in between. This structure is called the two-port resonator (Fig. 6b). If a single IDT is used for the input and output signals, the configuration is called the one-port resonator. There can also be some modifications in these configurations. In resonators, sensing layer can be deposited on to the IDTs and the impedance matching requirement is not as stringent because they have relatively smaller insertion attenuation. Also, the oscillation design is simple as this configuration offers relatively small phase change (~π) in the passband.

Both of these configurations have the same mechanism response and similar output characteristics Either of these configurations can be used to measure the changes in the phase velocity (v) and attenuation (α) of the acoustic waves upon exposure to gases. As the attenuation can suffer from undesired electromagnetic interferences, SAW sensor response is usually obtained in terms of velocity change to avoid such interferences. Experimentally, the velocity change is evaluated by measuring the shift in center (resonance) frequency (f) or phase (ϕ) of the wave. The measured changes in the centre frequency and the phase with and without gas exposure are related to the phase velocity as:

$$\frac{\Delta v}{vo} = \frac{\Delta \varphi}{\varphi o} = \frac{\Delta f}{fo}$$

where v_0, ϕ_0, and f_0 are the output velocity, phase, and centre frequency of the SAW wave in unperturbed state whereas v, ϕ, and f are those in perturbed states. In case of delay lines, it is necessary to measure small changes in the delay time. This can be accomplished by direct measurements of the pulse delay. However, the velocity changes are usually small enough that measurement of centre frequency or phase changes is more practical. The phase difference can be determined by using quadrature detection. On the other hand, a resonator configuration requires measuring its resonance frequency as the sensor response and relate it to the velocity change using Equation.

III. Temperature Dependencies

There are several notable factors that influence wave propagation in SAW and among all of them temperature is a critical one. The frequency of an acoustic device changes as a function of temperature which sets the foundation for developing SAW temperature sensors. There have been several diverse industrial applications of such sensor systems, for example in high speed/voltage motor engines, metallurgical vessels and others. SAW devices are workable at temperature as high as 600°C as reported in, however, with a chemical recognition interface, they can work at room temperature for chemical sensor applications. The quantitative relationship between temperature and resonating frequency may be expressed in Equation (1), i.e., by temperature coefficient of frequency (TCF). From the following equation, it is obvious that the TCF is associated with the fundamental frequency of a device:

$$Temperature\ Coefficient\ of\ Frequency\ (TCF) = \frac{1}{fo} X \frac{dfo}{dT}$$

Piezoelectric Material	Dielectric Constant	TCF [a] (ppm/°C)	Max. Working [b] Temperature	Velocity (m/s)	Comments
Quartz (ST-X)	3.8	0	573 °C	3159	Common and inexpensive, Stable against temperature, Not suitable in aqueous phase
$LiTaO_3$ (X-112° Y) $LiTaO_3$ (36° Y-X)	43	18 32	≈300 °C	3300 4160	High frequency SAW devices, Suitable for liquids phase operation, Temperature drifts
$LiNbO_3$ (128° Y-X) $LiNbO_3$ (64° Y-X) $LiNbO_3$ (Y-Z)	85.2	75 80 94	≈300 °C	3979 4742 3488	High frequency SAW devices, Suitable for SH-SAW liquid phase, Larger TCF values
AlN	8.5	19	≥1000 °C	5700	High frequency SAW devices and used in form of thin layer on other substrates, High thermal stability
$La_3Ga_5SiO_{14}$	18.23	≈0	1470 °C	2734	Enhanced piezoelectricity, High thermal stability Low insertion loss

Table 1. Comparison of different piezoelectric materials in terms of their dielectric constants, TCF, SAW propagation velocity and general comments for SAW manufacturing

Apart from resonating frequency, TFC values vary depending upon the nature of material and its cutting angle structure. From the Table 1, quartz is the most piezoelectric material, whereas LiTaO3 and LiNbO3 shows frequency drifts under temperature fluctuations. Gallium orthophosphate (GaPO4) and langasite (La3Ga5SiO14) possess high thermal stability. Aluminum nitride (AlN) is also a thermally stable piezoelectric material and shows a much higher SAW velocity compared to other piezoelectric materials. It is obvious that quartz has a zero TCF value showing its ability to remain stable against temperature variations during measurements. For chemical sensor applications frequency shifts due to temperature fluctuations needs to be avoided thus, piezo materials having low TCF are recommended. Furthermore, the problem of frequency shifts due to temperature variations during measurements can also be solved by integrating a suitable temperature compensation element, i.e., an additional SAW device as reference channel.

IV. Resonating Frequency and Sensitivity Relation

SAW resonators are well known for their exceptionally high frequency which makes them potentially suitable in mass sensing applications. The mathematical correlation between mass loading and the fundamental resonance frequency of piezoelectric materials was first explained by Sauerbery. This relation explains the frequency shifts as a result of mass loading taking into consideration all the important parameters of the substrate material. Equation (2) shows the frequency shift relationship with the fundamental resonating frequency for a typical SAW device:

$$\Delta f = -\frac{k \Delta m f o^2}{A}$$

In this equation, Δf is the frequency shift due to mass loading, fo is the fundamental resonance frequency, Δm is the loaded mass, A is the area and k is material constant. This shows that frequency response/shift due to mass loading increases as a function of the increasing fundamental resonance frequency of the device. The increase in frequency shift is parabolic. Unlike bulk acoustic wave devices, SAW resonators can be designed for much higher resonating frequencies i.e., from hundreds of MHz to the GHz range, which is significantly higher than quartz crystal microbalance (QCM). This feature makes SAW devices exceedingly favorable in sensing applications, with superior sensitivity, especially where dealing with trace analyte concentrations. Fig. 7 present the sensor responses of four different SAW devices for 1000 ppm of toluene, where all the SAW devices were coated with same recognition layer but having variable resonating frequencies starting at 80 MHz and going to 1 GHz. From this figure, it is clear that by increasing the fundamental frequency, the sensor response increases in a parabolic way, thus showing the experimental evidence for a frequency sensitivity relationship. While combining recognition layers with high frequency SAW resonators for sensing, the thickness of the coating material may be reduced down to monolayers, which results in a shorter response time due to a faster sorption-desorption process. Thus, increase in fundamental resonance frequency leads to enhanced sensitivity and, when combined with thin coatings, to shorter response times.

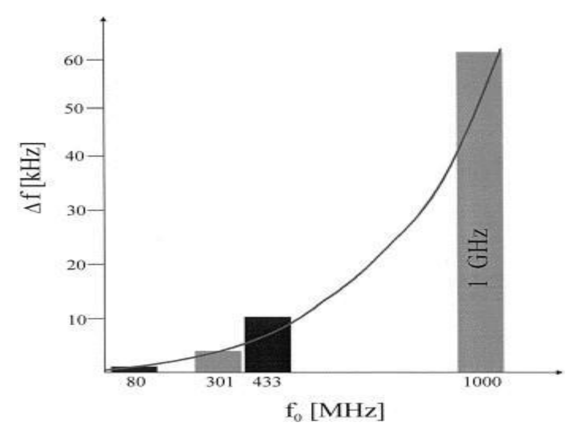


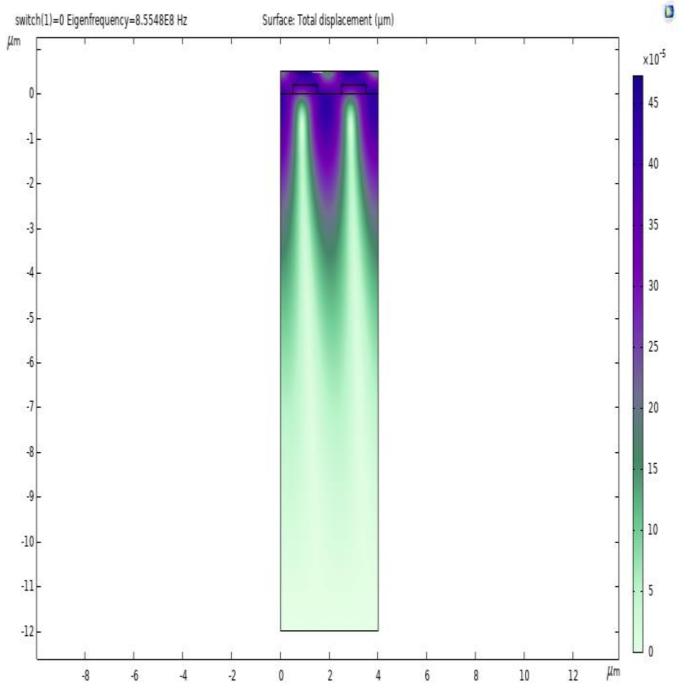
Fig 7. Sensor responses of different SAW devices for 1000 ppm of toluene. All the devices are coated with the same recogntion layer.

V. SAW GAS SENSOR SIMULATION

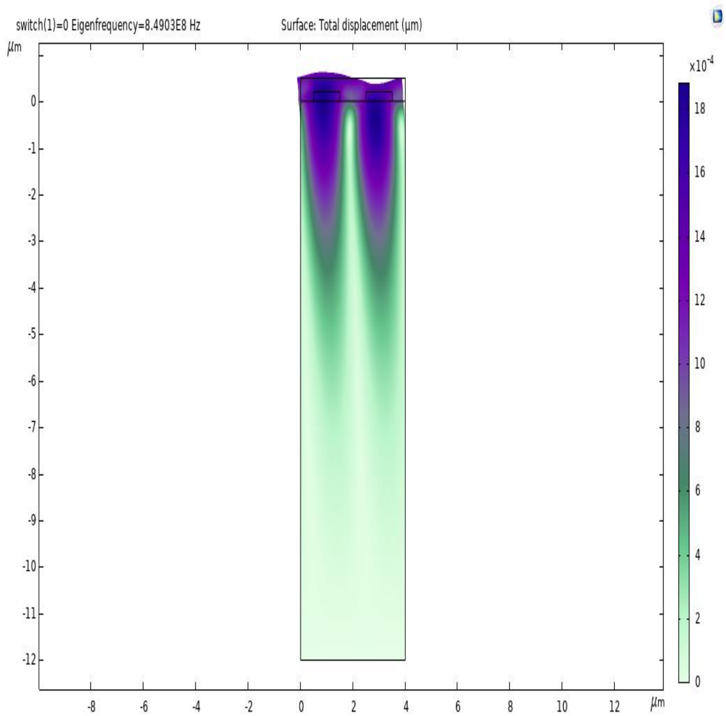
We have studied the SAW modes using anti resonance and resonance frequencies and the electric potential distribution characteristics on COMSOL 5.4 application.

Exposing the sensor to a 100ppm concentration of DCM in air leads to a resonance frequency shift of approximately 200 Hz downwards. This is computed by evaluating the resonance frequency before and after adding the density of absorbed DCM to that of the PIB domain.

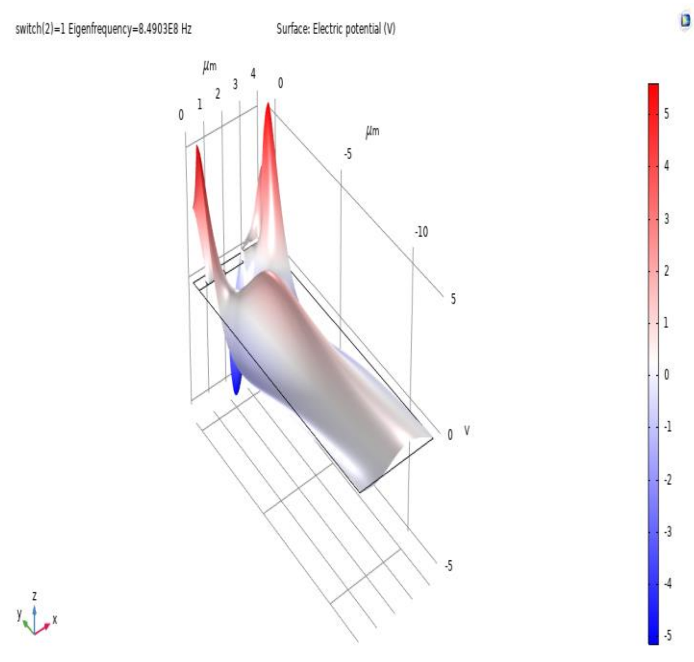
Note that the computational mesh is identical in both the solutions. This implies that the relative error of the frequency shift is like that of the resonance frequency itself. Thus, the shift is accurately evaluated despite being a few magnitudes smaller than the absolute error of the resonance frequency.



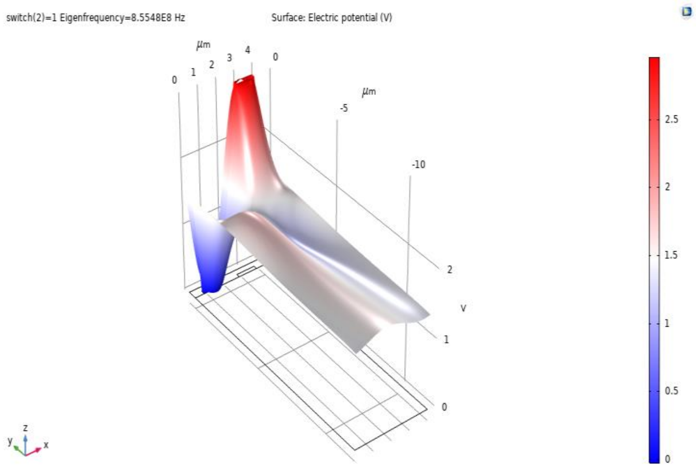
Deformed shape plot of the resonance SAW mode.



Deformed shape plot of the anti-resonance SAW mode.



Electric potential distribution and deformations at anti-resonance, anti-symmetric with respect to the center of each electrode



Electric potential distribution at resonance, symmetric with respect to the center of each electrode.

VI. REFERENCES

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