Modeling and Simulation of Surface Acoustic Wave Chemical Sensors

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ABSTRACT

In this paper, we present the design and modeling considerations of SAW (Surface Acoustic Wave) chemical sensors based on various structures. These sensors can be used for identifying environmental contaminants in large applications scale. Various finite element models of a Surface Acoustic Wave sensors are developed using CoventorWare and 3D analysis is performed on the devices to study the acoustic wave propagation and characterize the device. The effects of the various interdigital transducer (IDT) design, intermediate layer on the propagation characteristics is also investigated. Also, we present some results obtained from the device. Results indicate that with increasing the gas concentration the wave velocity decreases and the attenuation of the wave is reduced.

Keywords: chemical sensors, SAW, FEM, simulation.

1 INTRODUCTION

Surface Acoustic Wave (SAW) devices have been extensively used in gas sensors application mainly because these devices are relatively easy to fabricate (e.g. one of the simplest approach is by using commercially available SAW resonators and depositing chemical selective layer over the interdigital transducers) and because are highly sensitive. These devices have been used also as temperature, humidity and pressure sensors [1, 2].

Surface acoustic wave (SAW) sensors, which are sensitive to a variety of surface changes, have been widely used for chemical and physical sensing. All acoustic wave devices and sensors use a piezoelectric material (PVDF, guartz SiO_2, $LiTaO_3$, $LiNbO_3$, PZT) creates a mechanical stress. Piezoelectric acoustic wave sensors apply an oscillating electric field to create a mechanical wave, which propagates through the substrate and is then converted back to an electric field for measurement.

Two pair of symmetrical interdigital transducer (IDT) are the most usually used design for generating and receiving waves by exploiting the piezoelectric effect of the substrate as is illustrated in Figure 1. A SAW transducer consists of two interdigital arrays of thin metal electrodes deposited on a highly polished piezoelectric substrate. The electrodes that comprise these arrays alternate polarities so that an RF signal of the proper frequency applied across them causes the surface of the crystal to expand and contract. This generates the Rayleigh wave, or surface wave, as it is more commonly called [3].

In its simplest form, a SAW device appears as two comb-like metal structures deposited on a piezoelectric crystal surface (Figure 2 - Saw sensor part 1) and humidity sensing is reached by detecting changes in the sensitive layer which perturbing the surface acoustic wave channel.

The ability to control or compensate for the many surface forces has been instrumental in collecting valid data. In cases in which it is not possible to neglect certain effects, such as frequency drift with temperature, methods such as the "dual sensor" technique have been utilized (Figure 2 - Saw sensor part 2).

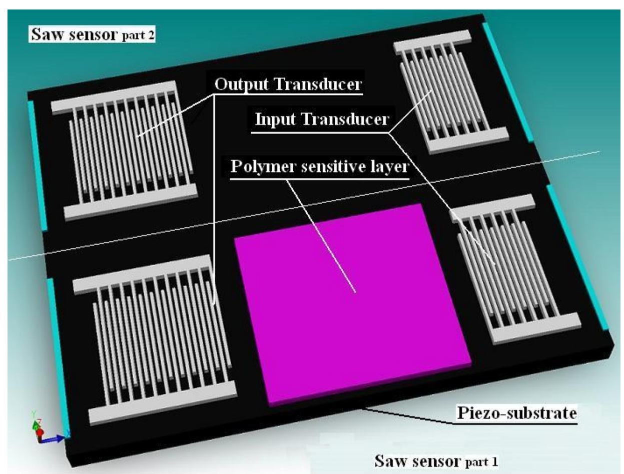

Figure 1: SAW-sensor structure.

Acoustic wave sensors are so named because their detection mechanism is a mechanical, or acoustic, wave. As the acoustic wave propagates through or on the surface of the material, any changes to the characteristics of the propagation path affect the velocity and/or amplitude of the wave. Changes in velocity can be monitored by measuring the frequency or phase characteristics of the sensor and can then be correlated to the corresponding physical quantity being measured.

De facto, all acoustic wave devices and sensors use a piezoelectric material to generate the acoustic wave.

Applying an appropriate electrical field to a piezoelectric material creates a mechanical stress. Piezoelectric acoustic wave sensors apply an oscillating electric field to create a mechanical wave, which propagates through the substrate and is then converted back to an electric field for measurement.

SAW devices can operate using a wide range of wave propagation modes: Rayleigh waves are the most common, but Lamb, Love, Bleustein–Gulyaev–Shimizu, Stonely, Sezawa, and other wave modes are employed [4].

In its simplest form, a SAW device appears as two comb-like metal structures deposited on a piezoelectric crystal surface - Figure 2, and chemical sensing is reached by detecting the mass loading when a desired chemical species binds with the coated selective layer and thus perturbing the surface acoustic wave channel.

SAW sensors are the most sensitive to mass loads. This opens up several applications including particulate sensors and film thickness sensors. If the sensor is coated with an adhesive substance, it becomes a particulate sensor; any particle landing on the surface will remain there and perturb the wave propagation. Particulate sensors are used in cleanrooms, air quality monitors, and atmospheric monitors.

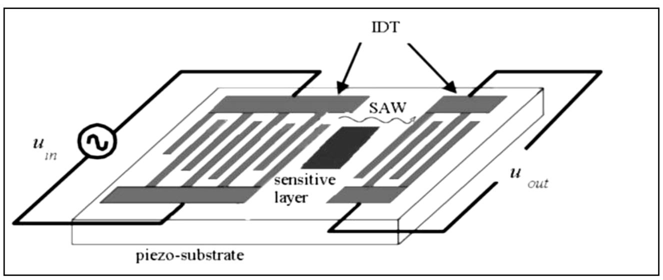

Figure 2: SAW device structure.

Generally there are three different types of SAW device structures: delay lines, one-port and two-port resonators. The two-port SAW resonators consist input and output interdigital transducers (IDTs) electrodes (comb-like metal structure) and reflection gratings (which can be fabricated using open or short metal strips). By applying sinusoidal signal at input port, acoustic waves are generated and propagate in piezoelectric layer in both directions. At the output port is converted back into an electrical signal. The reflector gratings minimize losses and create standing waves in a cavity [4]. The only difference for two-port delay line is that instead of reflectors there are acoustic absorbers and device works based on traveling time of generated wave at input transducer (transmitter) to output transducer (receiver). Figure 3 shows the typical structure of SAW resonators gas sensors.

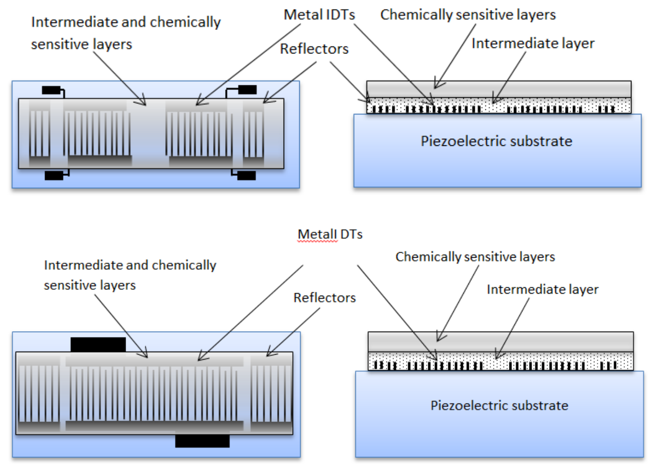

Figure 3: Top and cross-section view of standard two port (top) and one-port (bottom) SAW gas sensors.

2 SIMULATION

It is highly important to have methodology to model and simulate the device before the fabrication to fundamentally understand of the device performance. The simulation also helps to optimize design parameters and to overcome trials and fails. This was motivation to develop a three dimensional model for SAW devices.

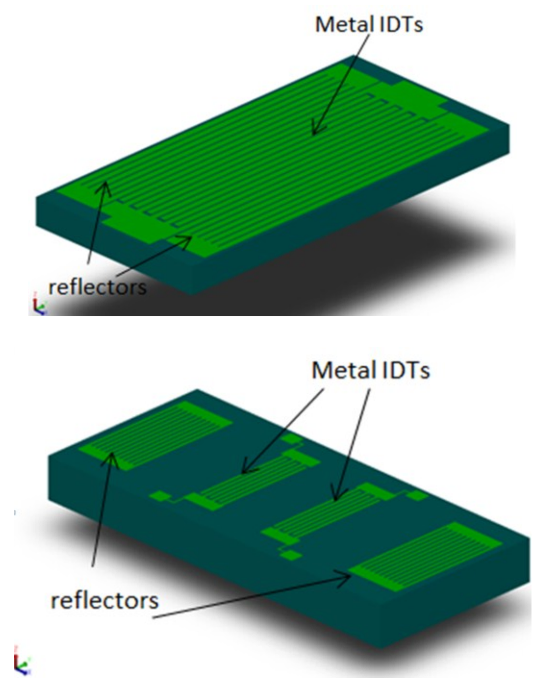

Figure 4: Simplified view of one-port (top) and two-port (bottom) SAW resonator model.

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Finite element analysis (FEA) was performed using CoventorWare micro-electromechanical systems (MEMS) design and simulation tool. Simplified model of one-port and two-port resonator is in Figure 4. The dimensions of the one-port piezoelectric substrate are 80µm in the X-axis, 120µm in the Y-axis and 10µm in Z-axis. The dimensions of the two-port resonator are 300µm in the X-axis, 100µm in the Y-axis and 10µm in Z-axis. The dimensions of model were chosen according to limitation of computational capacity as the real one-port SAW resonator has the dimension 700µm width x 1700µm length x 500µm thickness. The dimensions of the IDTs are 2.6µm the finger width and 1µm finger spacing, periodicity 7.2µm (2 x finger width + 2 x finger spacing) and aperture 70µm – for detail see Figure 5. The one-port resonator IDT has 8 finger pairs, the two-port resonator input and output IDTs has 3 finger pairs.

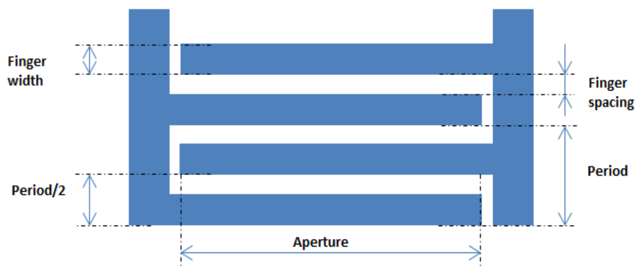

Figure 5: IDT dimension.

For simulation was in Preprocessor module set free tetrahedral meshing process. In MemMech module of CoventorWare was set piezoelectric analysis and on electrodes were applied potential of 1V (e.g. first and third electrode are set to 1V and second and fourth electrodes are zero potential).

3 RESULTS AND CONCLUSIONS

A 3D view of the wave propagation as results of the sinusoidal excitation of the devices is shown on Figure 6 and Figure 7.

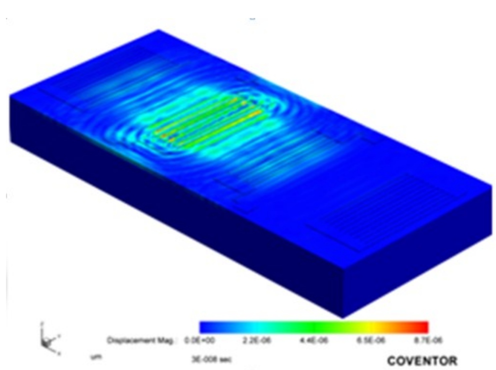

Figure 6: 3-D graphical represent showing acoustic wave propagation.

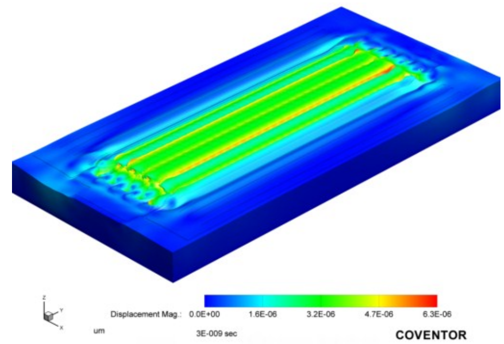

Figure 7: and 3-D graphical represent showing acoustic wave propagation.

The parametric analysis was performed for different thickness of intermediate layer, see Figure 8. As can be seen the highest total displacement is around the 0.5 thickness of ZnO intermediate layer and this would also result in highest sensitivity of SAW chemical sensor.

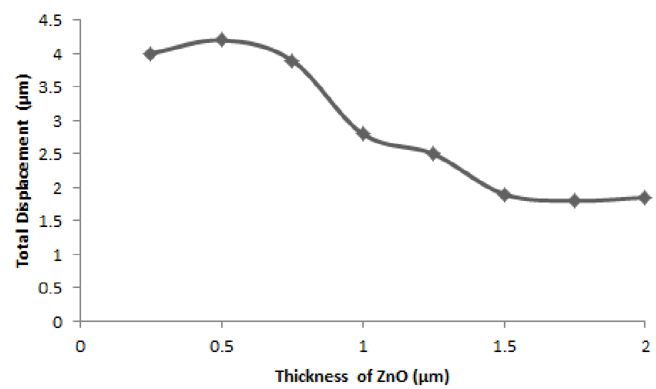

Figure 8: Total displacement for various thicknesses of ZnO intermediate layer.

The values of the modulus of elasticity and the density at different gas concentrations in chemical sensitive layer are utilized in the finite element model to determine the corresponding SAW gas sensor response. The lower detection limit for these SAW sensors lies in the range of a few ppb. The gravimetric SAW (and as well as QCM) detectors have the advantage of sensitivity, competitively priced and have a fast response time. The problem for SAW devices is their limited selectivity. The selectivity highly depends on the chemical selective coating layers which only allow specific gases to adsorb, unfortunately these specific coatings exist only for very few gases.

SAW sensors are very sensitive, but often respond to different parameters than surface mass that can affect the properties of SAW propagation. SAW devices are very sensitive to environmental factors such as temperature, humidity, and these factors are key challenges for the development of SAW-based chemical sensors. Figure 9 shows the spectral response when SAW sensor was exposed to 1% concentration of acetone.

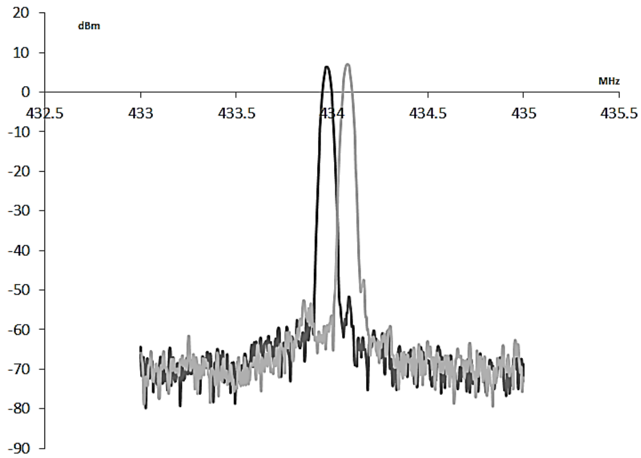

Figure 9: Spectral response when SAW sensor exposed to 1% concentration of acetone.

The SAW sensors are highly sensitive (but often respond to different parameters than surface mass that can affect the properties of SAW propagation) and often very selective, small, but robust, highly compact, portable, easy to use and relatively cheap devices. However there are no selectivity in presence of several interfering compounds or when analyzing complicated mixture. This can be solved by highly selective coating materials or by fabrication microsensor arrays of several SAW sensors coated with various chemoselective materials.

Results indicate that with increasing the gas concentration the wave velocity decreases and the attenuation of the wave is reduced and our methodology provides powerfull tools to tune optimal design parameters.

4 ACKNOWLEDGEMENT

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