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A Novel MEMS based Surface Acoustic Wave Gas Sensor for Carbon Dioxide Detection in Hot-Process Areas

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Abstract: The ever increasing applications of sensor networks is causing a growth in demand for low cost, energy efficient sensors for monitoring physical environment such as temperature, gas concentration or pressure. The paper presents a 3D model of a Surface Acoustic Wave Gas sensor for detection of CO_2 in high temperature areas. A robust and sensitive chemisensor has been realized by using the SAW phenomenon. In this study, nanostructures have been added in addition to the metallic layer to increase the surface to volume ratio of the sensor. The sensitivity of the sensor has been increased by using a piezoelectric material as a sensing layer. The choice of material absorption has been chosen by using Hard-Soft-Acid –Base theory, which is a relatively new concept to determine polymers for the active layer. The reliance of SAW reflection factor for unidirectional IDTs loaded by impedance on its resistive value was investigated. The sensor showed great results when exposed to varied concentrations of CO_2. Study also showed that langasite showed a stable frequency at higher temperature as compared to commonly used litium niobate. The design and simulation of the sensor is done using the Finite Element Analysis (FEA) module of COMSOL Multiphysics. The high temperature stability, fast response and robustness of the sensor showed promising industry applications.

Keywords: SAW; Sensor; Carbon Dioxide

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1. Introduction

Rising CO_2 levels are a major concern for nations worldwide. Apart from some serious consequences like global warming CO_2 levels in a room or indoor environment are also controlled with precision as an increase in the concentration to about 1000 ppm could cause nausea, headache and dizziness. Hot process areas like steel mills or Thermal Power plants where enormous amounts of CO_2 are generated as a result of combustion and thus it becomes essential to maintain a safe concentration limit. Monitoring of CO_2 in various working conditions has thus become a primary requirement for ventilation system designers. CO_2 being an inert gas, the design of a solid state room temperature sensor with sensor interface material is a great challenge for the designers and it becomes even more greater a challenge when the application is in hot process areas where materials have to withstand high temperatures and still give accurate readings. There has been a lot of research on building capacitive, metal oxide and NDIR based sensors in the past. Recently the focus has shifted to development of SAW based sensors. Surface Acoustic Wave sensors are Micro-Electromechanical Systems(MEMS) where an acoustic wave travels along the surface of a piezoelectric substrate. Interdigitated transducers(IDTs) are placed on the surface of a piezoelectric substrate to generate and receive the acoustic waves. The area between the generator and receiver IDTs is sensitive to surface perturbation like a loading mass. This area is usually coated with a chemically active species which reacts with the target molecule by adsorption. The rise of interests and development of manufacturing techniques in nanotechnology has made it possible for designers to increase the sensitivity of SAW sensors by integrating nanostructures on acoustic surfaces of the sensors, but introduction of these structures also changes the morphology of the piezoelectric substrate [1]. This change can cause significant changes in the wave propagation. Many studies and analysis have been conducted to understand the effect nanostructures have on the wave propagation, many models like the delta function model, coupling of mode model and Greens function model are very common. These models address certain design issues with respect to SAW filter design but they lack the ability to predict the full-scale behavior of the device. Finite Element Analysis(FEA) has the capability to address a lot of unsolved issues like second order effects in high frequency applications. FEA can help us solve three major questions that were previously difficult to resolve due to lack of CAD tools 1. Magnitude of increase in sensitivity obtained by integrating nanostructures on the SAW sensor surface? 2. Effect of nanostructures on the wave propagation. 3. Effect on the sensitivity by switching the conventional sensing layer with piezoceramic material? In our paper we propose the design and simulation a SAW sensor where we discuss how we could increase the sensitivity of the existing sensors.

2. Model consideration of the SAW sensor

2.1 Operating Principle

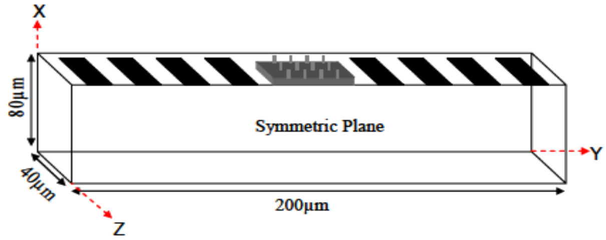
The SAW device configuration adopted in this study is the delay line structure, where two sets of electrodes are patterned on the surface of the piezoelectric substrate. A voltage signal is applied at the input electrodes, which by the converse piezoelectric effect is converted to mechanical perturbations on the surface. The acoustic wave propagates in the area between the two sets of electrodes. As the wave reaches the output set of electrodes the mechanical wave is converted into an electrical signal by the direct piezoelectric effect. In a piezoelectric material the propagation of the wave is governed by

$$T_{ij} = c^{E}_{ijkl} - e_{ijk} E_k$$

Here T represents the stress sensor, c^E the elasticity matrix, e the piezoelectric coupling constants, E_k the electric field intensity. This formula serves as the basis for building the geometry.

Figure 1. shows a schematic representation of a SAW sensor. In this study, a one-port delay line Saw sensor is considered. For SAW generation and propagation, a piezoelectric material- XY langasite is used, where Y-axis is the direction of propagation of the wave. The dimensions of the SAW device along the X, Y and Z axis are 80µm, 200µm and 40µm, respectively. To take advantage of the symmetric nature of the device we only consider the 2-D model for our analysis.

Figure 1. Cross-sectional Schematic of a typical FET based Biosensor.



An electrical signal is first applied to the IDE on the left which in turn generate an acoustic wave. The wave propagates along the Y direction close to the surface of the piezoelectric substrate. In this part of the study we intended to investigate the effect of adding nanostructures on the propagation and detection of the acoustic wave. The sensor here was designed to work at a frequency of 80µm. The operating frequency was found to be 300 Mhz. The design also included the electrodes to be placed 20µm apart from each other. Three reflectors were placed at either side of the sensors. Finally a block of air was created to simulate the atmosphere and was placed on top of the substrates. ZnO nanostrucutres were introduced to the detection area. Due to the 2D simplification, the cylindrical nanopillars were also simplified to small cylindrical structures with diameter 50nm. The height of the nanopillars was chosen to be 200nm as it is already determined to be an optimal height for nanopillars by Zhang [2]. The pillars were arranged in a simple array of 60 nanopillars spaced 1µm apart. The designed sensor was meshed and resulted in 48989 elements in the mesh.

2.2 Langasite Layer

Langasite is one amongst the recently investigated piezoelectric materials for high temperature applications. Its high melting point around 1,490 °C has made it very favorable choice for hot process area sensing. The first report on langasite noted that it could have zero temperature coefficient of the elastic vibration frequency near room temperature [8]. Hornsteiner et al. remarked on the advantages of langasite for high temperature SAW devices and reported a delay line operating up to 1,000°C. In a subsequent paper [9] they remarked on the increasing SAW attenuation with temperature and discussed the potential application as an ID tag (wireless mode). AlN [10] and other materials related to langasite [11,12] have also been considered for high-temperature SAW devices although it appears that much of the recent work directed at high-temperature sensing has used langasite. Surface transverse (SH) waves have been studied in langasite but mostly for resonator and liquid sensing applications. We will focus on Rayleigh (ordinary) surface waves. The surface wave velocity, temperature coefficient, electromechanical coupling coefficient, and power flow angle vary with the direction of propagation. The propagation direction is usually specified using the Euler angles Takeguchi et al. [11] reported that the (0°, 140°, 22°–24°) cut had zero temperature coefficient, zero power flow angle, and good electromechanical efficiency. In addition this direction yields a natural single phase unidirectional transducer. Based on experimental and theoretical investigations, Naumenko and coworkers recommended the orientation (0°, 138°, 27°) when also considering the anisotropy parameter, which determines the amount of diffraction. This particular cut has been used in much of the SAW sensor work to date.

2.3 Polymer Sensing Layer

The HSAB theory was developed by Ralph Pearson in the early nineteen sixties, in order to explain the different complexation behaviour of cations and ligands, the preferences of some compounds to react with other chemical species and their reactions mechanism [13]. According to this theory, hard Lewis bases prefer to bond to hard Lewis acid, and soft Lewis bases prefer to bond to soft Lewis acid. In some instances, a borderline Lewis acid may prefer to bond with a borderline Lewis base. Hard acids and hard bases exhibit some common features: low polarizability, high electronegativity. While hard bases hold their valence electrons tightly, hard acids do not contain unshared pair in their valence shell [14].Carbon dioxide is an example of hard acid (together with H+, Li+, Na+, $AlCl_3$, B(OR)3, Mg2+, Fe3+, etc.). According to HSAB theory, a hard base is suitable for sensing CO_2. Examples of hard bases include alcohols (ROH), ethers (R_2O), acetate anion (CH_3COO-), sulphate anion ($SO_4$2-), carbonate anion ($CO_3$2-), water (H_2O), ammonia (NH3), primary, secondary and tertiary aliphatic amines (RNH_2, R_2NH, R_3N). The interaction between hard acids and hard bases is mainly ionic, while the interaction between soft acids and soft bases is predominantly covalent. This aspect could be important for gas sensing, since mainly the hard acid - hard base tandem can ensure the reversibility of the reaction, and, thus, increased device lifetime. The HSAB theory may be used to select the sensitive materials for CO_2 molecules detection. For this reason, according to this rule, a simple organic molecule or a polymer which contains an amino group (that acts as hard base) can be a potential candidate for CO_2 sensing. A lot of literature data can be explained according to this theory. Different polymers sensitive toward CO_2 molecule such as BMPT, Versamide 900 [3-4], poly (3-aminopropyltrimethoxysilane octadecyltriethoxysilane copolymer (PA-POS) [5-7], poly (3-aminopropyl- trimethoxysilane propyltrimethoxysilane copolymer) (PAPPS)[6], polyethyleneimine [3], nanocomposites matrices based on polyallylamine and aminocarbon nanotubes, polyethyleneimine and aminocarbon nanotubes[8-10] are hard bases due to the amino groups which are present on their polymeric backbone. Small organic molecules which are sensitive to CO2 can be classified as hard bases according to HSAB. Among these sensitive layer, one can remind: 7, 10, dioxa-3,4 diaza-1,5,12, 16- hexadecatetrol (both oxygen and nitrogen atoms act as hard base), diamino-pmenthane, triethanolamine, tri-n-octylamine, 1-naphtylamine, benzylamine, dipropylamine, N,N, -bis(2hydroxiethyl)ethylenediamine. The selected compound for CO2 detection in SAW-BAW devices include aliphatic amines polymers such as: simple polyallylamine, N substituted polyallylamine, polydiallylamine and polyvinylamine and mixture of these polymers. All these polymers are hard bases, according to HSAB rule, and can interact at room temperature with CO2 molecules [14]. This interaction is an acid base equilibrium. The reaction is reversible and yields carbamates. In this paper we choose polyallylamine as the sensing layer as it is much more stable at higher temperatures.

3. Results and Discussion

In this paper we study the possibility of a one port Saw sensor whose geometry has been simplified so as to make the analysis easier. Figure 2 shows the simplified geometry of the sensor. The presence of the aluminum IDT electrodes and the langasite film cause the lowest SAW mode to split up in two eigen solutions, the lowest one representing a series resonance, where propagating waves interfere constructively and the other one a parallel ("anti-") resonance, where they interfere destructively. These two frequencies constitute the edges of the stopband, within which no waves can propagate through the IDT. The resonance and anti-resonance frequencies evaluate to approximately 439 MHz and 449 MHz, respectively. Exposing the sensor to a 100 ppm concentration of CO_2 in air leads to a resonance frequency shift to approximately 300 MHz downwards. This is computed by evaluating the resonance frequency before and after increasing the density of adsorbed CO_2 to that of the Langasite domain. Note that the computational mesh is identical in both these solutions. This implies that the relative error of the frequency shift is similar to 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. In a real setup, the drift is often measured by mixing the signal from a sensor exposed to a gas with a reference signal from one protected from the gas. The beat frequency then gives the shift. The Figure 3. shows a pictorial representation of the meshed elements which does not contain the IDT as it is not involved in the deformation study as it is the source of the signal.

Figure 2. Simplification of a one port SAW sensor

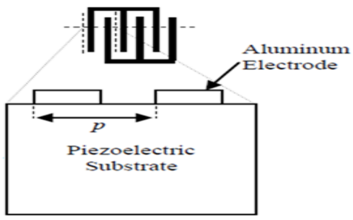
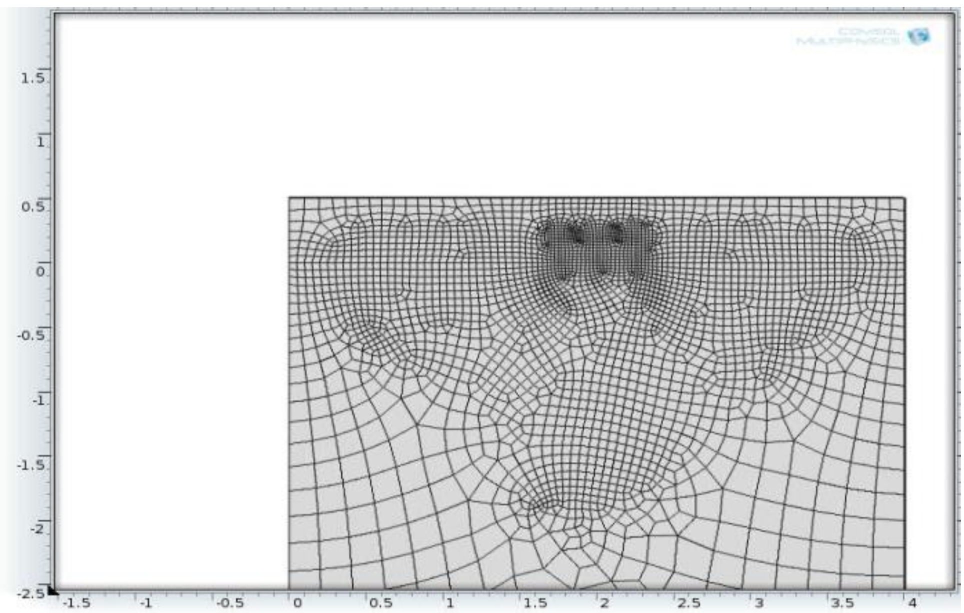
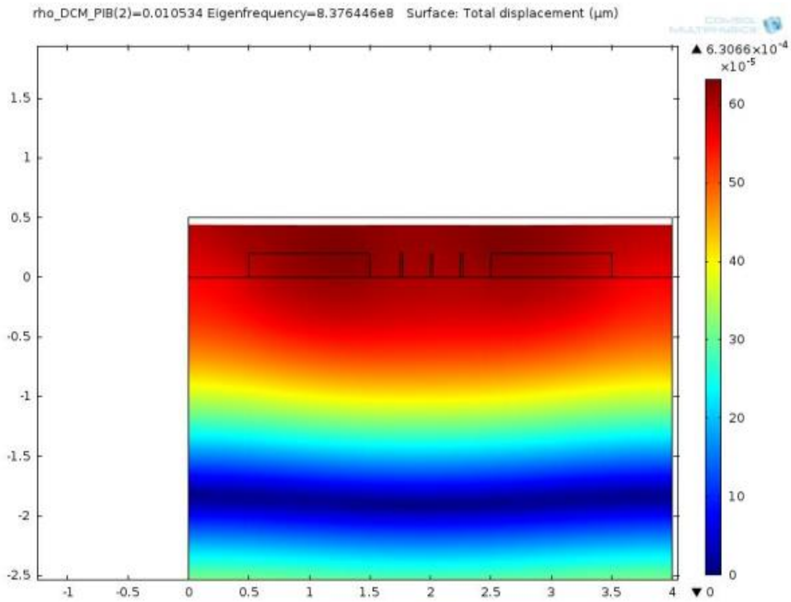


Figure 3. 48989 meshed elements.



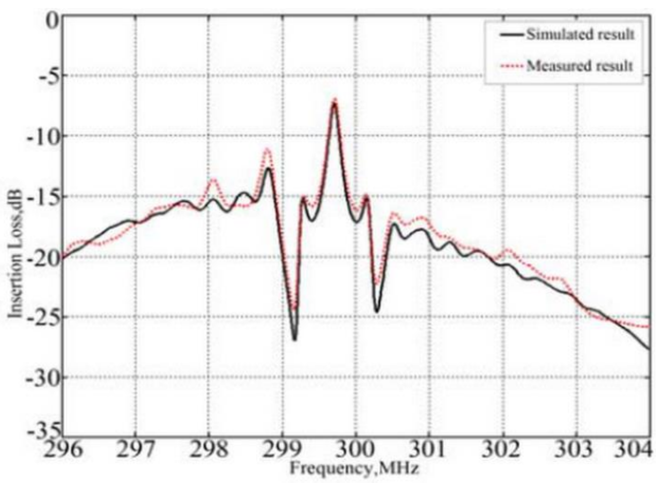
The displacement plot of the surface is represented by Figure 4. Figure 5 shows a typical response profile obtained from four consecutive 60 seconds on-off exposures to 5% of CO_2 in pure air at 25^{o}C and 1atm to investigate the repeatability of the gas sensor. ~ 2 kHz of sensor response was observed from 5% CO_2 detection. Also, it can be noted that four gas exposures are in good reproducible run. The values of SAW responses shift from average value within ±3%. Thus, the short-term repeatability of the SAW sensor response toward CO_2 can be considered excellent. Further work will be done on the sensor performance as sensitivity and detection limit.

Figure 4. Deformed shape plot of the resonance SAW mode.



(1)

Figure 5. Frequency response of the sensor.



4. Conclusion

A 300 MHz SAW based gas sensor incorporating differential resonator-oscillator structure with excellent frequency stability was simulated. One-port SAW resonators on a same Langasite substrate with low insertion loss, high Q-value, and single resonation mode were fabricated for the feedback element of the oscillator. Excellent medium term frequency stability (h) of ±25 Hz/h was measured. The possibility of using different geometry of nanostructures for increasing the adsorption surface area could provide room for improvement in the proposed design. Use of sensing layers apart from polyallylamine can also provide scope for future research as using an even more stable polymer could increase the longitivity of the sensor.

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Conflicts of Interest

The authors declare no conflict of interest.

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