Available online at www.elixirpublishers.com (Elixir International Journal)

Advanced Engineering Informatics

Elixir Adv. Engg. Info. 40 (2011) 5138-5140

3D Modeling of a surface acoustic wave based sensor

N.J.R. Muniraj¹ and K.Sathesh²

¹Tejaa Shakthi Institute of Technology for Women, Coimbatore, India ²Department of ECE, Karpagam College of Engineering, Coimbatore, India.

ARTICLE INFO	ABSTRACT	
Article history:	To develop a 3D computational model of a Surface Acoustic Wave based sensor in order to understand the SAW wave propagation characteristics built with enhanced sensitivity. A Surface Acoustic Wave (SAW) is an acoustic wave propagating along the surface of a	
Received: 17 August 2011;		
Received in revised form:		
17 October 2011;	solid material. SAW's are featured in many kinds of electronic components including filters,	
Accepted: 26 October 2011;	oscillators, sensors, etc. SAW devices typically use electrodes on a piezoelectric material to	
	_ convert an electrical signal to a SAW and back again. In this model we investigate the	
Keywor ds	resonance frequencies of a SAW gas sensor, which consists of an Inter Digitated Transducer	
Inter Digitated Transducer (IDT),	(IDT) etched onto a piezoelectric LiNbO3 (Lithium Niobate) substrate and covered with a	
LiNbO3 (Lithium Niobate),	thin Poly Isobutylene (PIB) film. The mass of the PIB film increases as PIB selectivity	
Poly Isobutylene (PIB) film,	adsorbs CH2Cl2 (Dichrolomethane, DCM) in the air. This causes a shift in resonance to a	

slightly lower frequency.

© 2011 Elixir All rights reserved.

Introduction

CH2Cl2 (Dichrolomethane, DCM).

Surface acoustic waves are elastic waves which propagate along the surface of an elastic body while dying out exponentially into the bulk of the body. Surface acoustic wave (SAW) sensors are micro electro mechanical (MEMS) systems in which the 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 very sensitive to surface perturbation like mass loading. A SAW device consists of a piezoelectric material (or film) on which interdigitated transducers (IDT) are placed. Usually, a single SAW device operates as an input and an output transducer. This makes it possible to create an acoustic wave by applying an voltage signal and vice versa. His property makes SAW devices interesting for applications allowing it, e.g., to operate as an analog electric filter at selected frequencies (in the range from about 10 MHz to 2.5 GHz). SAW devices are also widely used in mobile phone technology, wireless communication and telecommunication systems, etc. In this model we have LiNbO3 as a substrate. Upon the substrate we then add silicon IDT electrodes and PIB film. This causes 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 adsorption of DCM gas is represented as a slight increase of the density of the PIB film. The sensor is exposed to 100 ppm of DCM in air at atmospheric pressure and room temperature.

Model consideration of a saw gas sensor

A SAW-device usually consists of a Piezoelectric material with several interdigitated transducers. To ease modeling, a periodic structure is assumed, where only a section of the SAWstructure is modeled. The SAW devices are used because it

Tele: <u>E-mail addresses: njrmuniraj@yahoo.com, sathesh_kce@yahoo.com</u> © 2011 Elixir All rights reserved operates at a high frequency (MHz GHz) -high resolution, high sensitivity, Room temperature operation, Can work on a wireless platform .Can work in both dry and aqueous environments (eg: gas sensors, biosensors).

Saw gas principle

The simplest SAW device consists of a polished piezoelectric crystal, named lithium niobate (LiNbO3), with two Interdigitized Transducers. The latter are made of a thin metal layer, of silicon, deposited by means of evaporation.

When an a.c signals applied to the bus bars of the input IDT, the resulting electric fields between adjacent fingers produce mechanical deformation in the piezoelectric crystal. At a resonant frequency, the effect of each of the IDT fingers adds constructively, and a wave is produced which propagates away from the transducer in both directions. Half the input energy will therefore propagate across the distance between the two transducers, and reach the output IDT.



Figure 1: SAW gas sensor

Figure 1 shows the IDT electrodes (in black), the thin PIB film (light gray), and the LiNbO3 substrate (dark gray). For the sake of clarity, the dimensions are not to scale and the IDT has fewer electrodes than in common devices.

A slice of the geometry is removed to reveal the modeled unit cell (in white) Figure 2 shows a simplified piezoelectric SAW-device section of length L and height h. On the [010] surface inter digitized transducers apply positive and negative voltages of equal amplitudes in an alternating manner. The piezoelectric domain is referred to as Ωp while boundaries with positive or negative IDT's are denoted $\partial \Omega +$ and $\partial \Omega$ -, respectively. The boundaries at the [100] and [(-1)00] surface are referred to as $\partial \Omega p$ while other faces are represented by $\partial \Omega n$.



Figure 2: Simplified SAW-device

IDTs used in SAW devices may have hundreds of identical electrodes, and each electrode can be about 100 times longer than it is wide. You can therefore neglect the edge effects and reduce the model geometry to the periodic unit cell shown in Figure 3.





The height of this cell does not have to extend all the way to the bottom of the substrate but only a few wavelengths down, so that the SAW has almost died out at the lower boundary. In the model, this boundary is fixed to a zero displacement

Results and discussion

The presence of the aluminum IDT electrodes and the PIB film cause the lowest SAW mode to split up in two eigensolutions, 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 stop band, within which no waves can propagate through the IDT. The resonance and anti-resonance frequencies evaluate to approximately 842 MHz and 858 MHz, respectively. Figure 5.1 and Figure 5.2 show the corresponding SAW modes.

Figure 5.3 and Figure 5.4 show the electric potential distribution characteristics for these solutions.

Exposing the sensor to a 100 ppm concentration of DCM in air leads to a resonance frequency shift of approximately 162 Hz downwards. This is computed by evaluating the resonance frequency before and after increasing the density of adsorbed DCM to that of the PIB 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 which is of 162 Hz.

Simulation Results



Figure 5.1. Deformed shape plot of the resonance SAW mode







Figure 5.3. Electric potential distribution and deformations at resonance, symmetric with respect to the center of each electrode



Figure 5.4. Electric potential distribution at anti-resonance, anti-symmetric with respect to the center of each electrode. Applications of saw gas sensor

SAW devices are widely used in today's modern high frequency communication systems due to their stability and reliability even in the GHz region. A single SAW device operates as an input and an output transducer.

SAW devices are also widely used in mobile phone technology, wireless communication and telecommunication systems, acoustically induced charge transport, light storage, modulation of photonic structures optically cavities and the driving of micromechanical systems.

Conclusion

Thus, a MEMS based SAW gas sensor for the study of wave propagation characteristics was designed using COMSOL multiphysics (Version 4.1) and the simulation was done considering various materials such as Tungsten, Molybdenum, Silicon & Lead zirconate titanate electrodes. Among them Silicon has a better frequency shift of 162 HZ, whereas Tungsten has 624 HZ, Molybdenum has 529 HZ and Lead zirconate titanate has 784 HZ.

The 'Silicon' material does not react with oxygen and will not have any effect if placed in the atmosphere. This is one of the major advantages of using Silicon as electrodes. On using Silicon electrodes the Resonance frequency shift decreases rather than using other material electrodes like Tungsten, Molybdenum & Lead zirconate titanate. This does not make much difference in the frequency of the original signal (before the exposure of DCM) even when the mass of PIB is increasing, during the exposure of sensor in DCM.

References

1. Ahmadi and Zirarah, (2004). "Characterization of multi- and single-layer structure SAW sensor", *Sensors 2004*, *Proceedings of IEEE*, vol. 3, pp. 1129–1132,

2. Atashbar, M.Z, Bazuin, B.J, Simpeh, M, Krishnamurthy, S., (2005) 3D FE simulation of hydrogen SAW gas sensor, *Sensors and Actuators B*, 111-112, 213-218.

3.Auld.B.A, (1990) Acoustic Fields and Waves in Solids, vol. 1&2, 2nd edition. Krieger Publishing Company.

4.Brigati.S, F. Francesconi, F. Maloberti, C. Melano Protti, and M. Poletti, (1997) "A VLSI full custom general purpose gas sensor interface", Proceedings of IEEE International Conference on Electronics, Circuits, and Systems (ICECS `97), Cairo, Egypt, pp. 1490-1493.

5.Ho .K and che chan.H (2003)., "Development of a Surface Acoustic Wave Sensor for In-Situ Monitoring of Volatile Organic Compounds", *Sensors* vol. 3, pp. 236–247.

6.Rao, Y.L, Zhang, G., (2006). Enhancing sensitivity of SAW sensors with nanostructures, Current *Nanoscience*, In Press.

7.A.Venemaa, E. Nieuwkoopa, M.J. Vellekoopa, M.S. Nieuwenhuizenb and A.W. Barendszb(1986), "Design aspects of saw gas sensors".

8. Willatzen. M, (2001) Ultrasound transducer modeling – general theory and applications to ultrasound reciprocal systems, *IEEE Transactions on Ultrasonic's, Ferroelectrics, and Frequency Control*, 48, 100-112.

Specification	Value	Materials
р	101.325[kP]	Air pressure
Т	25[degC]	Air temperature
R	8.3145[Pa*m^3/(K*mol)]	Gas constant
c_DCM_air	100e-6*p/(R*T)	DCM concentration in air
M_DCM	84.93[g/mol]	Molar mass of DCM
K	10^1.4821	PIB/air partition constant for DCM
rho_DCM_PIB	K*M_DCM*c_DCM_air	Mass concentration of DCM in PIB
rho_PIB	0.918[g/cm^3]	Density of PIB
E_PIB	10[GPa]	Young's modulus of PIB
nu_PIB	0.48	Poisson's ratio of PIB
eps_PIB	2.2	Relative permittivity of PIB

Table 1: Material Definition