High Frequency SAW Resonator Design, Simulation, and Optimization With Applications to Chemical Gas Sensors

Libin Sun [(1)], Mona E. Zaghloul [(1)]

(1) School of Engineering and Applied Science, The George Washington University, Washington, DC, 20052, http://www.gwu.edu

Abstract

Surface Acoustic Wave (SAW) resonators with high resonant frequency (in the GHz range) are described. In this work Interdigital Transducers (IDTs) of the SAW resonator are scaled down to 150nm. The resonant frequency of a SAW resonators is mainly limited by the width of IDTs and types of piezoelectric materials used. Hence, hundreds nanometer size of IDTs will increase the frequency up to several Gigahertz (GHz), which will improve the sensitivity to detect a small load mass change in real time and shows a promising potential for sensing fields.

1. Introduction

The study of the surface acoustic wave (SAW) was first published by Lord Rayleigh in 1885[1]. He described the behavior and properties of acoustic waves propagate on the plane surface of elastic solid. In 1959, the relation between the shift of the resonant frequency and the alter of the load mass on one of the piezoelectric materials, quartz, was figured out by Sauerbrey[2]. Then in 1965, White and Voltmer published the technique that direct deposit a periodic array of metal that works as electrodes on the face of the piezoelectric layer, which helps to propagate the surface acoustic wave and build the first SAW device[3]. Their method makes it possible to form the electronic signals by applying the electronic field to those IDTs and transforms those signals to surface acoustic waves[3].

Currently, most of the Surface Acoustic Wave sensors are working from 25MHz to 1000MHz [4], [5], [6]. To design a SAW resonator with high sensitivity, we need to promote the operating frequency. Besides the type of piezoelectric materials, the major limitation to increase the resonant frequency is the size of the IDTs. With the advanced Nanoscale facility at the clean room, and with the help of Voyager, and Pioneer (Electric Beam Lithography equipment), it is possible to implement the IDTs array scaling the width of IDTs down to 150nm [7]. This motivates us to research the scaling the dimension of SAW resonator to acquire higher mass sensitivity.

In this paper, the design, simulation, and optimization of SAW resonators are introduced. We start the simulation in the sequence of 2D single unit model, 3D single unit model, and 3D entire model. First, we use 2D single unit model to prove that 150nm size of IDTs can improve the resonant frequency. Then, build the 3D single unit model to measure the sensitivity of load mass. Finally, we run the simulation with the complete SAW resonator 3D model. Additional, to optimize the SAW resonator sensitivity performance, we simulate the device with several different piezoelectric materials including lithium niobate ($LiNbO_3$), zinc oxide (ZnO), quartz (SiO_2), aluminum nitride (AlN) and lead zirconate titanate ($Pb(Zr_x,Ti_{1-x})O_3$), or PZT-4). In Nordin paper [4], an entire one port resonator with the width equal to 900nm that was realizing as a filter. To verify our simulation results, we built the design in [4] with the same boundary conditions and compare the simulation results with measurement results obtained in [4]. All the simulations were done with 3D Finite Element Analysis (FEA) on the COMSOL Multiphysics 5.2 [8] platform and the data results are processed in MATLAB.

2. Simulation of SAW Resonator

2.1 Geometry and Boundary Conditions

The figure 1 where is a) b) show the dimension and notation for each boundaries of entire structure of one port resonator. As showed in figure 1 c), the layers from the bottom to the top are the substrate, piezoelectric layer, IDTs and mass bulk. The dimension of the structure is listed in table 1. The length of entire structure equal to $2L + 4Nd1 + 2nd1 - d1$.

Table 2 shows the mechanical and electrical boundary conditions for the entire structure. To apply the external voltage, we set the β_V (Left five connected IDTs) as terminal, and β_G (Right five connected IDTs) as ground in electrical boundary conditions. The terminal type set as voltage and value is equal to 1V. All the rest of the boundaries are set as Free for the Solid Mechanics interface and set as Zero charge for the Electrostatics interface.

We use free tetrahedral to mesh the model. Since the piezoelectric displacement is mainly generated close to the IDTs, we increase the number of domains around IDTs and decrease the number of domains in rest field to improve the simulation efficiency. The complete mesh consists of 21409 domain elements, 8934 boundary elements and 3275 edge elements as demonstrated in the figure 1 a).

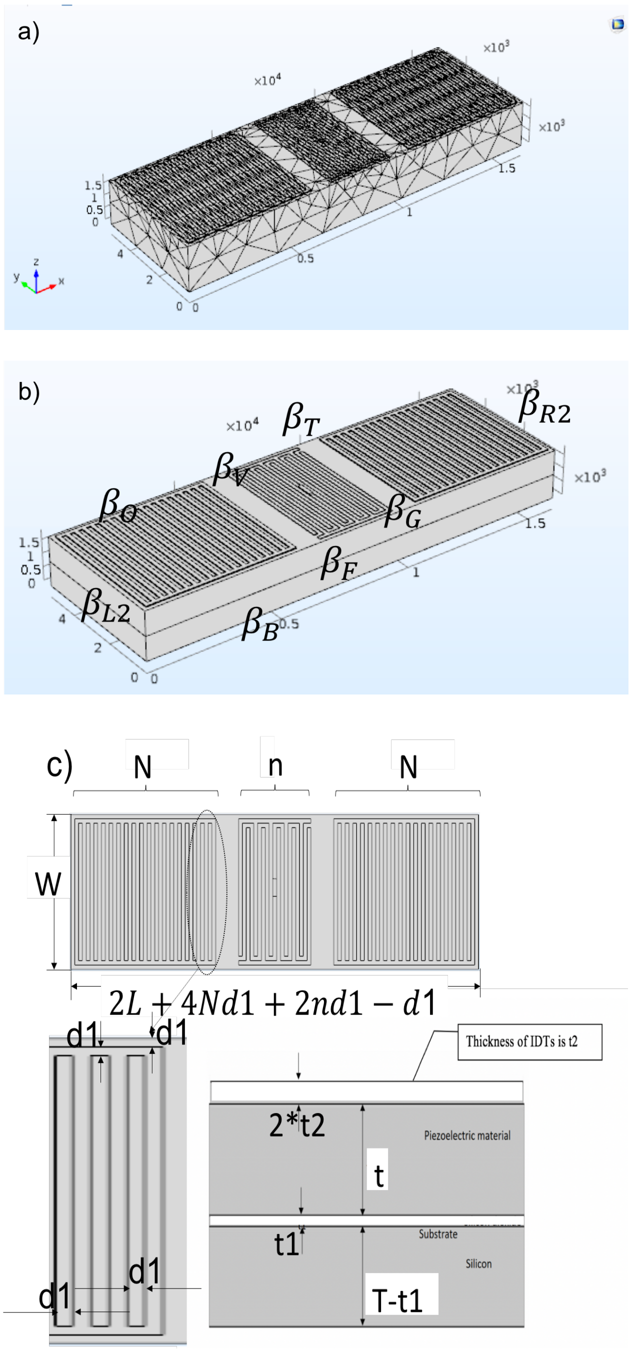

Figure 1. a) The mesh of the resonator; **b)** The notation of each boundary of entire structure of one port resonator; **c)** The top view and side view of the resonator.

Table 1. Dimension of the entire one port resonator

Name	Expression	Description
d1	0.15 [um]	Periodic distance of interdigital fingers
W	5 [um]	Width of aperture
N	19 [um]	Number of fingers in the reflectors
L	0.9 [um]	Distance between reflector and transducer
n	10 [um]	Number of fingers in the transducer
t	0.9 [um]	Thickness of piezoelectric layer
t1	0.18 [um]	Thickness of sio2
t2	0.02 [um]	Thickness of IDTs
t_PIB	0.05 [um]	Thickness of PIB thin film

Table 2. Mechanical and electrical boundary conditions for entire structure of one port resonator.

Boundary	Mechanical Boundary Conditions	Electrical Boundary Conditions
β_TTop of the absorption layer (PIB)	Free	Zero charge
β_B Bottom of the piezoelectric layer	Fixed constraint	Zero charge
β_{L2}, β_{R2} The left and right sides of the piezoelectric layer and absorption layer	Periodic layer	Periodic layer
β_F, β_O The front and back sides of the piezoelectric layer and absorption layer	Periodic layer	Periodic layer
Piezoelectric layer	Piezoelectric material	Charge conservation, Piezoelectric
β_VLeft five connected IDTs		Terminal (Type: Voltage, 1V)
β_GLeft five connected IDTs		Ground

In this work we would like to measure the sensitivity of the device when coated by absorbing material to absorb the gas molecules. To measure the sensitivity of the device, we coated the device with polyisobutylene (PIB) thin film, which has a high selectivity to absorb the CH_2Cl_2 (dichloromethane, DCM) from air [9]. The density of the PIB thin film is set as switch*ρ_PIB kg/m^3, where switch is the parameter used to multiply the density of the PIB, and the ρ_PIB is the density of the PIB equal to 918kg/m^3. Hence, for the entire structure of one port resonator, the mass of the PIB thin film equal to M1

$$M1 = (t\_PIB \times 4d1 \times d1) \times \rho\_PIB \times switch$$
$$= 4.131 \times 10^{-18} \times switch\ kg \qquad (1)$$

where t_PIB and 4d1*d1 are the thickness and the area of the PIB thin film, respectively.
The load mass is controlled by the parameter “switch”.

2.2 Simulation Results

For $LiNbO_3$, Figure 2 shows the surface displacement of entire one port resonator. According to the simulation results that list in table 3, with the load mass change 4.131×10^{-20}kg, the resonate frequency shift 1453Hz. As the load mass change about 4.131×10^{-21}kg, the resonate frequency shift about 145 Hz.

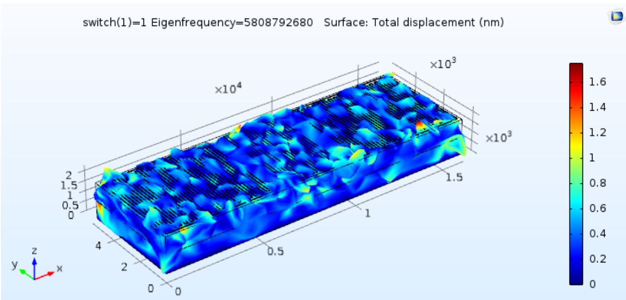

Figure 2. The resonant frequency and totally surface displacement of 3D entire resonator with $LiNbO_3$.

Table 3. The Frequency versus displacement with different load mass for $LiNbO_3$.

Switch	Resonator frequency(GHz)	Load mass (kg)	Compare to switch =1	
			Δf (Hz)	Δm (kg)
1	5808792680	4.131×10^{-18}	0	0
1.01	5808791227	4.17231×10^{-18}	1453	4.131×10^{-20}
1.001	5808792535	4.135131×10^{-18}	145	4.131×10^{-21}

The simulation results of all five materials (lithium niobate, zinc oxide, quartz, aluminum nitride and lead zirconate titanate) are listed at table 4.

Table 4. Comparison of the one port resonator with different materials.

Material	Resonant frequency (Hz)	Load mass difference (kg)	Frequency shift (Hz)	Displacement (nm)
$LiNbO_3$	5.808792×10^9	4.131×10^{-21}	145	35.54
Quartz	5.104999×10^9	4.131×10^{-20}	2661	7.51
ZnO	6.364431×10^9	4.131×10^{-20}	1000	23.02
PZT	4.273802×10^9	4.131×10^{-20}	996	21.86
AlN	9.9881799×10^9	4.131×10^{-21}	928	3.906

3. Conclusion

The simulation results prove that with the width of IDTs scaling down to 150nm, the resonant frequency can be improved to about 9.988 GHz (with AlN). In addition, for one port resonator designed in this account a high sensitivity, is obtained. A frequency shift of about 928Hz with the load mass modify 4×10^{-21}kg (with AlN).

4. References

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