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Different Bulk acoustic wave resonator designs for high frequency applications

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Abstract

The high growth of the various radio frequency (RF) systems, e.g. mobile telecommunication, satellite communication and other wireless devices that accrues high frequency range and the racing for minimizing the devices size makes Micro-electromechanical systems dominate the interests of all manufacturers, but the biggest limitation is that not all technologies are compatible with integrated circuits (IC) manufacturing process. MEM's devices that are based on acoustics waves like SAW (surface acoustic wave) and BAW (bulk acoustic wave) overcome this limitation with outstanding performance.

BAW resonator is a new technology raised during the last decade shows promising results as it operates in higher frequencies 0.9-5.5GH and has a good temperature stability over SAW, Better selectivity, IC manufacturing process compatibility, and lower insertion loss. However, BAW resonators still needs optimization to achieve the high quality factor also the temperature dependency is still a big problem.

Lateral energy leakage is the main key for determining the quality factor of BAW. Using the concept of the short circuit can force the wave to be reflected back to the active region and prevent the wave to be lost outside providing high quality factors. Also using thin film bulk acoustic wave resonator (FBAR) instead of solidly mounted resonators (SMR) strength this concept all these results in what called air-like FBAR. Also the thickness and material of the piezoelectric and electrodes play a very important role in determining the resonance frequency for BAWs. In this work there will be intense study on all of these parameter to choose the best for the design Also, using

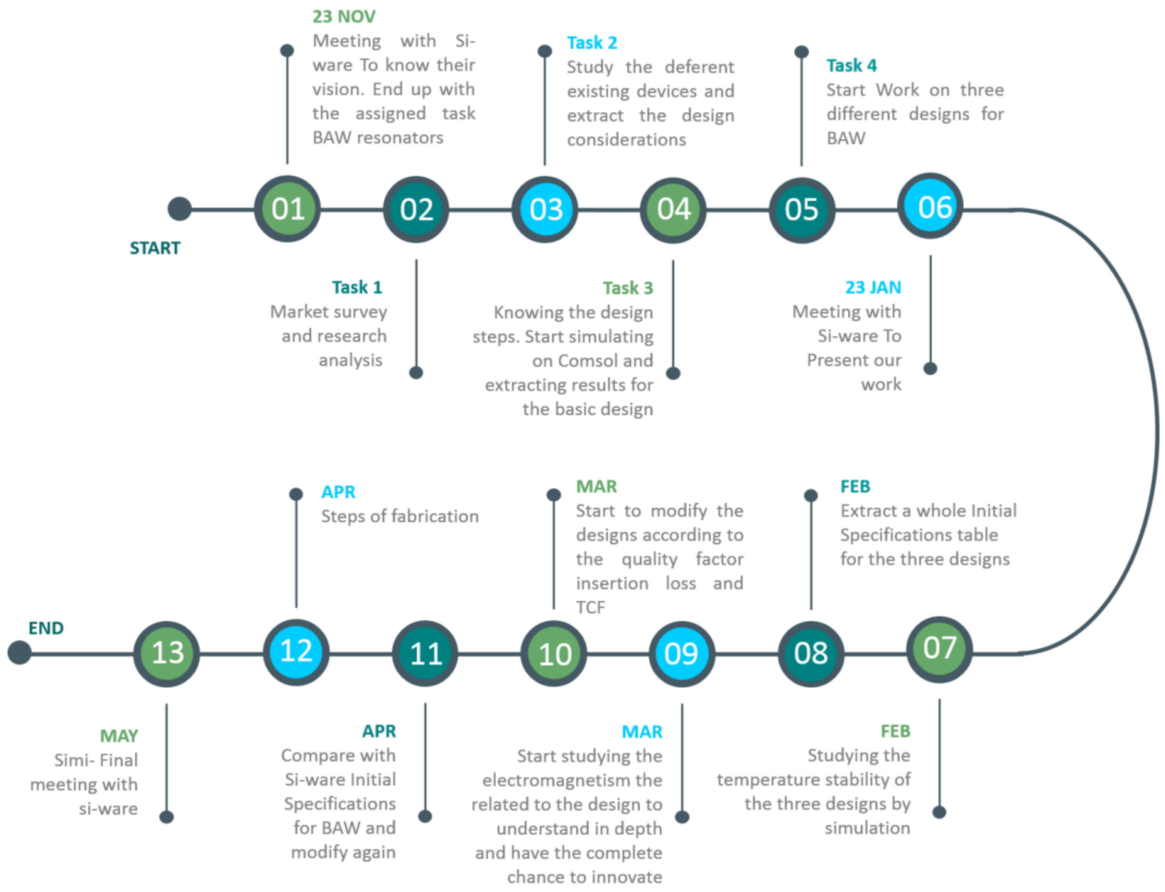
BAW resonators and CFR filters are discussed here with their detailed electrical model, design considerations and the materials used. FEM simulations using COMSOL software are done clarifying three designs for the three concepts, with detailed information to carry such simulations, In addition, Cadence is used to electrically model the three designs

Finally this work will present the upcoming plane for developing BAW for a seek of developing an existing BAW resonators manufactured by Silterra Malaysia (1)

Acknowledgements

We have been very interested to search and work in this topic. We worked those few months with each other, searched a lot, asked all doctors and engineers around us and met to discuss again and again trying to understand and reach to the right information. We would like to express our sincere gratitude to our advisor Professor Hassan Mustafa for his guidance and support. We would also like to thank Eng. Ayman for all the discussions and helpful advice throughout this project. Also, we would like to thank Eng. Kirollos Ernest, Eng. Ahmed Samy, Eng. Moez El-Massry for their helpful discussions and suggestions. We would like to thank everyone who helps us in this work

Time management chart



23 NOV
Meeting with Si-ware To know their vision. End up with the assigned task BAW resonators

Task 1
Market survey and research analysis

Task 2
Study the deferent existing devices and extract the design considerations

Task 3
Knowing the design steps. Start simulating on Comsol and extracting results for the basic design

Task 4
Start Work on three different designs for BAW

23 JAN
Meeting with Si-ware To Present our work

FEB
Studying the temperature stability of the three designs by simulation

FEB
Extract a whole Initial Specifications table for the three designs

MAR
Start studying the electromagnetism the related to the design to understand in depth and have the complete chance to innovate

MAR
Start to modify the designs according to the quality factor insertion loss and TCF

APR
Compare with Si-ware Initial Specifications for BAW and modify again

APR
Steps of fabrication

MAY
Simi- Final meeting with si-ware

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Chapter one : Introduction

Needing a new functions to an existing device or material is not the only key to the innovation, now days the racing to develop the small devices with a big efficiency leading to the most important key factor which is the integration of new functional materials into silicon microsystems MEMS devices. On another side, Wireless communication systems had the most interest now due to the rising of IOT (Internet of things) concept in all the life fields , the biggest limitation of these systems is that not all their technologies are compatible with integrated circuits (IC) manufacturing process.

Microwave MEMS devices that depend on acoustic waves like SAW (surface acoustic wave) resonators and BAW (surface acoustic wave) resonators overcome this limitation, Also, as the size of the devices is usually directly related to the wavelength of the electromagnetic wave at a certain frequency, which at the same time is directly related to the propagation velocity of the electromagnetic wave, acoustic waves which has a propagation velocity less than that of electromagnetic waves about 4 or 5 times resulting in a device size lower in the same proportion(1).

Until 90's the main resonators elements used in communication applications with a reasonable frequencies range up to 2 GHz and stable band were the crystal and ceramic resonators but they were off chip elements, Compared to SAW based technologies which enable the usage of smaller devices but they were used only in low frequency communication applications and a lot of previous fabrication processes were not combatable with IC manufacturing process. All these leads to the need for a technology that can overcome all these limitations

BAW Acoustic resonators can be found in data transfer (e.g. Bluetooth , WLAN), global positioning systems (GPS, Galileo), satellite communications, cellular mobile systems and many other applications(2). the interest to this technology can be sum up to the device size, cost and performance.

Beside all the benefits of the acoustic resonators in general, the growing use of mobile communication systems that operate at radio frequencies (RF), need sharp, small, band-pass filters and oscillators and require to transmit or receive signals within a certain bandwidth at a specified frequency and suppress all other signals within a small device calls for a new generation of resonators.

1.2. Overview

1.2.1. Acoustic Resonators

The main key phenomena in the acoustic resonator is the piezoelectricity which is a characteristic of the material that enable generating an electric field from applying a force (stresses and strains) to the material and vice versa. (4) Among the available piezoelectric materials, AlN and ZnO seem to be the most suitable for microwave applications due to their high acoustic propagation velocity and electromechanical coupling coefficient which can be defined as an intrinsic property of piezoelectric materials which relates the amount of converted electrical energy into mechanical energy or vice versa. (7)

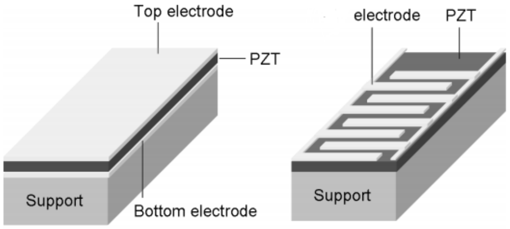


Fig 1.1 left: Surface Acoustic Wave Resonator.
Right: Bulk Acoustic Wave Resonator (7)

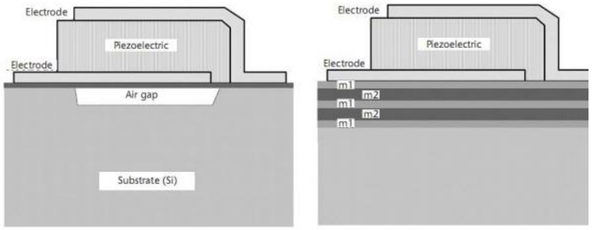


Fig 1.2 left: film bulk acoustic resonators (FBAR).
Right: solidly mounted resonators (SMR) (6)

Depending on how the acoustic waves behave in the piezoelectric material, two different technologies can be defined. First, Surface Acoustic Wave that depends on the lateral direction of the wave which means that it is propagate parallel piezoelectric and along the surface, they operates around 1.1GH and commonly manufactured on a LiTaO3 or LiNbO3 crystal substrates which are not compatible with the IC technology.(5) Second is Bulk Acoustic Wave that depend on longitudinal direction of the wave where the wave propagates inside the piezoelectric material Specially speaking in the thickness direction. They operates around 2-10 GHz and they are totally compatible with the IC technology. Fig.1.1 represents the two resonators, the advantage of SAW over BAW is only the simplicity of manufacturing, and this work will mainly focus on BAW resonators.

1.2.2. BAW (Bulk Acoustic Wave) Resonators

But Why BAW? For frequencies above 2 GHz which is needed in telecommunication technology (3G and 4G) as well as other wireless applications, SAW resonators can’t achieve the requirements of insertion loss, pass-band and power handling control, besides that, SAW resonators are very temperature sensitive so it loses their achieved quality factor quickly with the temperature. In BAW the stress on the electrode is not as high as in SAW so it will extent to handle high frequency and power applications with high performance. (6)

The simplest BAW structure is illustrated in fig.1 where a piezoelectric material is sandwiched between two metal electrodes which are deposited on the substrate, the wave must be confined for the resonance of the device, and among the confinement method BAW has two categories - fig.1.2 - : film bulk acoustic resonators (FBAR) and solidly mounted resonators (SMR). The driving idea for both is to make reduce the losses of the wave into the substrate, for FBAR, the air gab act as a short circuit which force the wave to reflect only between the two electrodes, for SMR the Bragg reflector consists of an alternating low and high acoustic impedances layer which confines the acoustic wave between the electrodes. The only advantage of SMR over FBAR is the better mechanical handling but still FBAR provide a better quality factor.

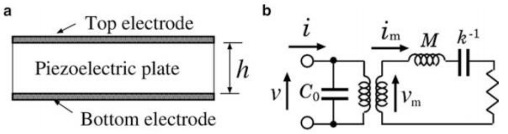


Fig.1.3 left: Bulk Acoustic Wave Resonator. Right: the coupling between electrical and pizoelectrical (8)

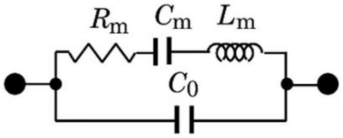


Fig.1.4 Electrical equivalent circuit model (BVD model) (8)

1.3. Project Motivation and Objectives

Now days, Micro-electromechanical systems (MEMS) has a big impact on much more application than in the past which allows the inventions of new types of sensors and actuators. This always leads to more complex functions that rises by itself a new problems and challenges, most of these limitations can be overcome by adding a variety of functional materials onto silicon. Piezoelectric materials which can convert signals from mechanical to electrical and vice versa. piezoelectric materials (PZT) is an important family of functional materials, beside that, many of the PZT materials have a well-established fabrication techniques and it is suitable for miniaturization, The successful integration of piezoelectric and micro fabrication techniques will enhance the sensing and actuating properties. This process will be a lead toward the development of novel MEMS devices. However, BAW resonators still needs optimization to achieve the high quality factor. Not only the losses of the wave outside the piezoelectric will negatively affect the quality factor also as it based on the longitudinal direction only, the lateral propagation of the wave is undesirable (spurious modes) and the temperature dependency is still a problem. (10)

This work seeks to develop a BAW design with high quality factor, low insertion loss and a good temperature stability compared to an already existing design from Si-ware Company, verified by Comsol and Cadence simulations. In order to achieve these goals, the specific objectives are as follows:

1- Investigate a good BAW design according to the specifications mentioned above with Q factor higher than 2000
2- Developing the design to eliminates the spurious modes and enhance TCF
3- Verify all the used techniques by analytical model
4- Develop finite element model for the design in 1D and 3D
5- Compare the design with Si-ware establish design and develop again.

This work will focus only on BAW resonators as mentioned previously and apart this first chapter dedicated to the introduction, overview, motivations and objectives of this work, the report is structured as follow:

Chapter 2 will introduce CRF Design. **Chapter 3** will introduce W/AlN/W resonator design. **Chapter 4** will introduce ZiO2 resonator design

Finally, a summary of the results from this work along with some potential future Recommendations

Chapter Three : W/AlN/W FBAR

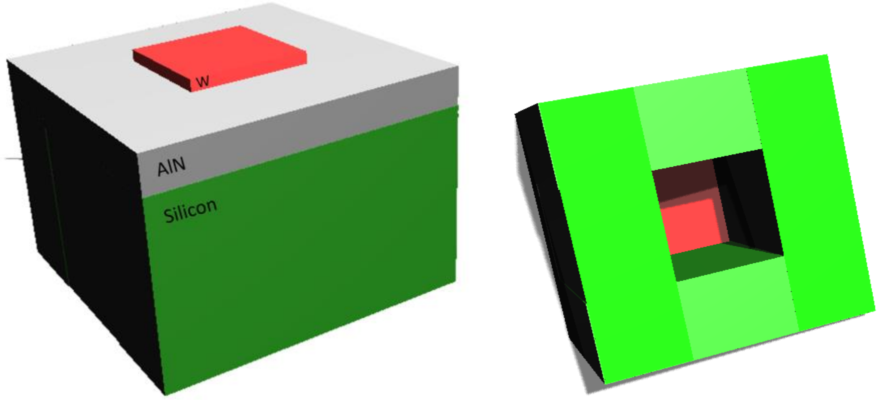


Fig 3.1 Left: 3D outside view for W/AlN/W design. Right: 3D inside view for the design

3.1 Introduction

Lateral energy leakage is the main key for determining the quality factor of BAW. Using the concept of the short circuit can force the wave to be reflected back to the active region and prevent the wave to be lost outside providing high quality factors. Also using thin film bulk acoustic wave resonator (FBAR) instead of solidly mounted resonators (SMR) strength this concept all these results in what called air-like FBAR. Also the thickness and material of the piezoelectric and electrodes play a very important role in determining the resonance frequency for BAWs.

The design proposed -fig 3.2- in this chapter is based on FBAR technology which use the air gap to confine the wave in the piezoelectric. The operating frequency of the resonator is 2.4 GHz

In this chapter there will be intense study on all of these parameter to choose the best for a FBAR design as follows

Section 3.2: Basic Concepts of FBAR, how does the wave behave, how does the piezoelectric act, and Sources of quality factor loss in FBAR

Section 3.3: The electrical modeling of FBAR how to get electrically the quality factor and the effective coupling coefficient

Section 3.4: the proposed design with Full Comsol multiphasic 5.3.a and Cadence simulations

Section 3.5: Suggestions to a higher Quality factor and how to eliminate the unwanted lateral modes

Finally, a summary of the results obtained with this design is compared to Si-ware specifications along with some potential future Recommendations

3.2. Basic Concept of FBAR

The basic structure of FBAR is simply a piezoelectric layer sandwiched between two metal electrodes in which the wave propagate between them with an air gap underlying the bottom electrode. Acoustic wave is excited by an alternating volt source between the two electrodes which result in an electromagnetic waves and converted to acoustic wave by the means of piezoelectric material. Unlike the electromagnetic waves, acoustic wave needs a medium which there will be two propagation direction: (i) thickness direction longitudinal and (ii) lateral shear direction. Any lateral wave propagation consider unwanted modes that affect negatively the quality factor ("a parameter of an oscillatory system or device, such as a laser, expressing the relationship between stored energy and energy dissipation")[7].

Piezoelectric effect – Fig 3.9 - is the coupling between the electric and mechanical properties, and only the materials with special symmetry class of crystal structure can support this effect.

So, FBAR generates resonance frequency by converting the electromagnetic waves into mechanical waves via piezoelectric material.

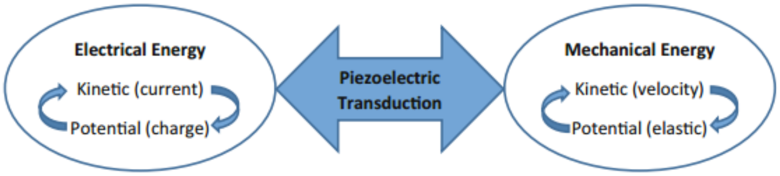


Fig 3.9 A block diagram representing the energy flow in a piezoelectric resonator

3.3. FBAR Electrical Model:

The simplest model that can model the propagation in a piezoelectric material is a plate with thickness h which will have its fundamental resonance frequency when Y → 0 at

$f= \frac{nV}{2h}$ eq. 3.1

where V is the acoustic wave velocity, and n is an integer called the order of resonance modes [4]

That lead us to the simplest model of BAW by considering two parts: (i) the piezoelectric material (ii) two parallel electrodes that form a capacitor C0, which means the we can predict the resonance frequency electrically fig.3.7 .

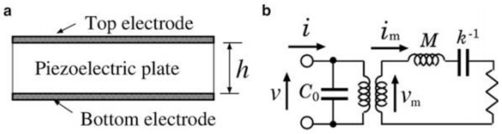


Fig.3.7 left: Bulk Acoustic Wave Resonator. Right: the coupling between electrical and pizoelectrical (8)

The simplest known electrical model is the Butterworth–Van Dyke (BVD) circuit model fig.3.8 where Cm, Lm, and Rm are the motional capacitance, inductance, and resistance, respectively and C0 is the clamped capacitance which expresses the electrostatic coupling between two electrodes.

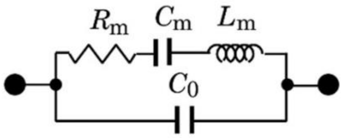


Fig.3.8 Electrical equivalent circuit model (BVD model) (8)

The following relations is well reported in the literature that can drive all BVD model as well as the quality factor and Effective coupling coefficient

At Y → ∞ (resonance frquency) the coupling coefficient is defined by :

$k^2{}_{eff} = \frac{\pi^2}{8}(\frac{{\omega_r}^2-{\omega_a}^2}{{\omega_a}^2})$ eq 3.2

And the quality factor

$C_o = \varepsilon_o \varepsilon_r \frac{A}{d}$ eqn. 3.3

$C_m = C_o \left[\left(\frac{\omega_s}{\omega_p}\right)^2 - 1\right]$ eqn. 3.4

$R_m = \frac{L_m \omega_m}{Q_m}$ eqn. 3.5 $L_m = \frac{1}{C_m {\omega_m}^2}$ eqn. 3.6

$$Q = \frac{\omega}{2} . \frac{C_m V^2 + C_0 V^2 + L_m {I_2}^2}{R_m {I_2}^2 + R_0 {I_1}^2}$$

The quality factor can be get by many ways the most traditional one is the 3D-badwidth

There many other electrical equivalent models like Mason's Equivalent Circuit Model (9) which are more accurate and take into account the losses in the piezoelectric and the damping loses in general, But for simplicity this work use BVD for model BAW in Cadance.

3.4. Material and thicknesses:

3.4.1. Electrodes

The only way to choose the electrodes material is to look into the material acoustic impedance. Choosing material with high acoustic impedance means that the material can prevent the losses of the wave outside the active region and confine the wave with high efficiency which will improve both the quality factor and the coupling coefficient. Tungsten (W), Aluminum (Al) and Molybdenum (Mo) are the most used material in BAWs as they have high acoustic impedance, table 3.1 summarize some of these materials' properties found in [1] that also will be used in simulations. The table shows that W has the highest acoustic impedance makes it the preferable for the design

Material	Acoustic impedance (kg/m^2.s)	Density (kg/m^3)	Acoustic Velocity (m/s)
W	101	19350	5230
Al	17.7	2700	6572
Mo	63.1	10200	6250

Table 3.1. Some if the interested Electrodes materials properties

3.4.2. Piezoelectric

Following equation (*****), the main key in selecting the resonance frequency is the material and the thickness. The chosen material should have high temperature stability, high longitudinal propagation velocity, low acoustic loses with high coupling coffceint and compatible with IC. All these parameters are material properties that are well reported prevousily. ZnO and AlN coming in the top of peio-electric material the compromise all of these properties. Table 3. 2 [2][3] is reported in the literature shows the important properties for aluminum nitride (AlN),zinc oxide (ZnO), lead zirconate titanate (PZT) and the crystal cadmium sulfide (CdS), among all of these material AlN has the highest velocity propagation and low acoustic loses, on the other hand it is clear that it has the lowest Piezoelectric coupling factor but its compatibility with IC manufacturing process and its well-known fabrication process [4] that can provide a high quality thin AlN films, makes it the most suitable material for BAWs. Also, the high longitudinal velocity makes AlN can be used in very high frequency range which is the scope of this work.

Material	**Longitudinal Velocity (m/s)**	**Density (kg/m^3)**	**Coupling Factor**	**IC Compatibility**	**Intrinsic Losses**
AlN	11050	3260	6.1%	Yes	Very Low
ZnO	6350	5610	9.1%	No	Low
PZT	4600	7500	35%	No	High
CdS	4500	4820	2.4%	No	High

Table 3.2. Some if the interested piezoelectric materials and crystals properties

To start work with AlN, all the material properties should be cleared and known, these values will either be used in analytical analysis and Comsol Simulations. In literature it has been found that the most used ratios for a mechanical damping is 0.25% and for dielectric loss is (0.005 -0.01).

Also, from [4][5] all the material properties can be summarize in three matrices :

(i) Dielectric matrix (permittivity) [$\times 10^{-11}$ F/m]: $\begin{bmatrix} 8 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 9.5 \end{bmatrix}$

(ii) Elasticity matrix (stiffness) [$\times 10^{-11}$ N/m^2] : $\begin{bmatrix} 3.45 & 1.25 & 1.2 & 0 & 0 & 0 \\ 1.25 & 3.45 & 1.2 & 0 & 0 & 0 \\ 1.2 & 1.2 & 3.95 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.18 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.18 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.1 \end{bmatrix}$

(iii) Piezoelectric constant matrix [C/m]: $\begin{bmatrix} 0 & 0 & 0 & 0 & -0.48 & 0 \\ 0 & 0 & 0 & -0.48 & 0 & 0 \\ -0.58 & -0.58 & 1.55 & 0 & 0 & 0 \end{bmatrix}$

3.4.3. Thickness

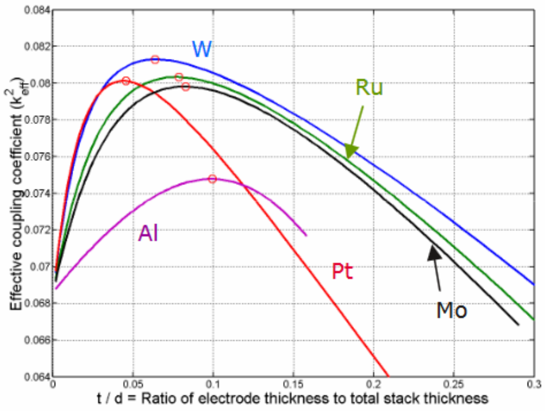


Fig 3.1 Effective coupling coefficient as a function of electrode thickness for a symmetric membrane AlN resonator. Typical electrode materials (Al, Mo, Pt, Ru and W) have been analyzed [6]

Butting all together, a stack of W/AlN/W was choosing for the design, which is meant to deliver high acoustic wave confinement, high coupling coefficient and high quality factor. But the specifications of the design doesn't only depend on the material selection it also depend on the thickness of each material used in the device. In [6] a full derivation to relate the effective coupling coefficient k_{eff} with the thickness and the material used, shown in Fig 3.1 which represents the effect of the ratio between the thickness of the two electrodes and the piezoelectric material on the coupling coefficient, the best ratios for different electrodes material relative to AlN film.

3.3 W/AlN/W resonator design dimensions

From equation (***** 2.39) and for a resonance frequency of 2.4GHz the Effective coupling coefficient can be calculated and from Fig 3.1 the best ratio between the thickness of the electrodes to the thickness on the piezoelectric is 0.1, fig 3.3 clarify all the dimension used.

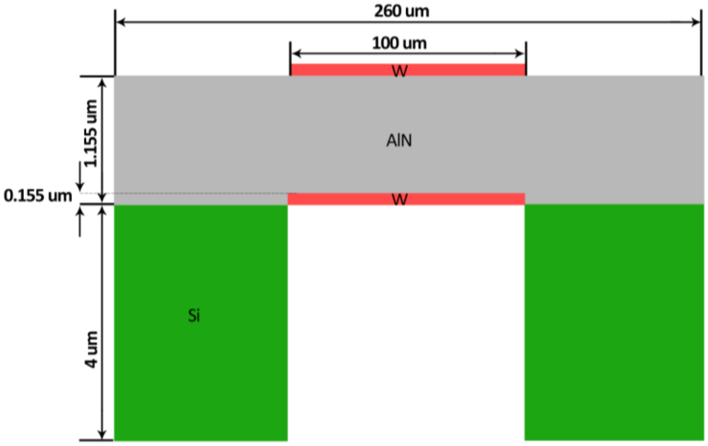


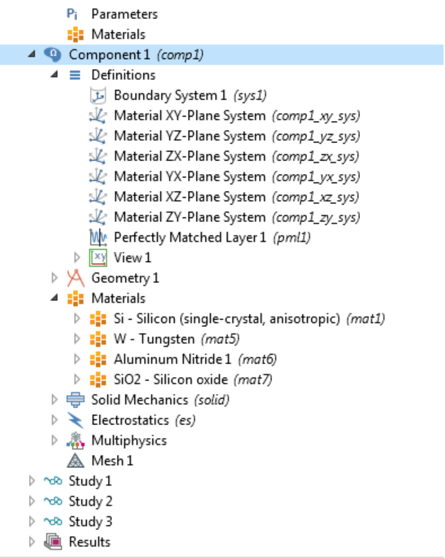
Fig 3.3 2D model for FBAR W/AlN/W with full geometry details

3.4 FEM Simulation

A fully simulation have been done using COMSOL 5.3.a to simulate the chosen dimensions and materials and to extract the resonance peak at the admittance curve, the temperature stability using the Eigen-frequency, the fundmental resonance mode shape and finally the quality factor.

3.4.1 Set the environment

Start with piezoelectric module which contain by default two physics (structure mechanics and electrostatics), build the design shown in Fig 3.3. A 3 um PML (perfectly matched layer) is added on the both sides of the design to eliminate any error du to any reflected wave and a fixed boundary from the structure mechanics physics is defined at the bottom of the Si substrate, a mesh is set to physics control mesh, the materials are added and Finally, parameter T is defined with initial value 300 [K]



- Parameters
- Materials
- Component 1 *(comp1)*
  - Definitions
    - Boundary System 1 *(sys1)*
    - Material XY-Plane System *(comp1_xy_sys)*
    - Material YZ-Plane System *(comp1_yz_sys)*
    - Material ZX-Plane System *(comp1_zx_sys)*
    - Material YX-Plane System *(comp1_yx_sys)*
    - Material XZ-Plane System *(comp1_xz_sys)*
    - Material ZY-Plane System *(comp1_zy_sys)*
    - Perfectly Matched Layer 1 *(pml1)*
    - View 1
  - Geometry 1
  - Materials
    - Si - Silicon (single-crystal, anisotropic) *(mat1)*
    - W - Tungsten *(mat5)*
    - Aluminum Nitride 1 *(mat6)*
    - SiO2 - Silicon oxide *(mat7)*
  - Solid Mechanics *(solid)*
  - Electrostatics *(es)*
  - Multiphysics
  - Mesh 1
- Study 1
- Study 2
- Study 3
- Results

Fig 3.4 shows the Model Builder after set up all parameter, studies and physics

All the properties mentioned on section 3.4.2 is defined in each material section, 100um is defined as the out-of-plan distance. The simulation shows three different analyses. In the first step, one can compute and investigate the Eigen-modes of the structure and in the second step the frequency response of the resonator is analyze within the desired bandwidth of 1.5 GHz to 3 GHz with step of 0.01. And finally a pre-stressed Eigen frequency study is added **Fig** 3.4 with the same setting for the eigenfrequncy study to show the response of the design with different temperatures (T).

3.4.2 COMSOL Simulation results

3.4.2.1 Study 1: Eigen Frequency

Fig 3.5.a shows the lowest Eigen mode which accrues at 2.4018 GHz which is fundamental longitudinal thickness mode and the operation frequency which the peak of the resonance at admittance should match. Note that COMSOL Multiphasic computes complex valued Eigen frequencies where the imaginary part gives a measure of the damping due to structural loss, polarization loss and anchor loss here there is no imaginary part which means that there is no losses at the resonance frequency in contrast with any other random unwanted mode that has loses around 0.001.

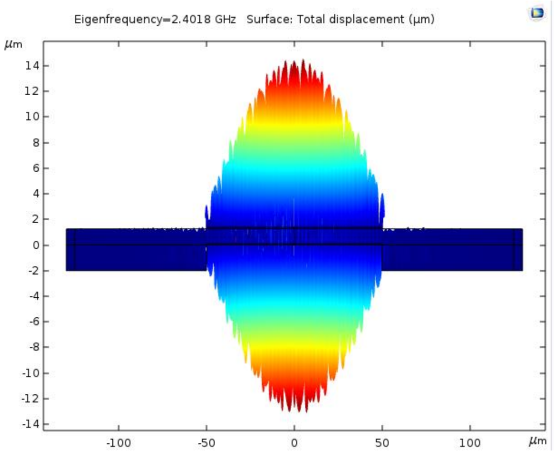


Fig 3.5 The lowest bulk acoustic mode of the resonator identified from the solutions of the eigenfrequency analysis

3.4.2.2 Study 2: Frequency domain

Fig 3.6 shows the absolute value of admittance as a function of frequency. Within the investigated range of 1.5 GHz to 3GHz, Note that the highest peak in admittance occurs at the lowest BAW mode of 2.4018 GHz.

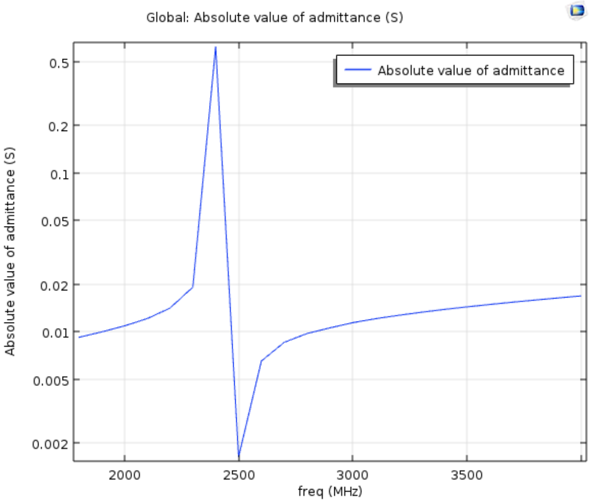


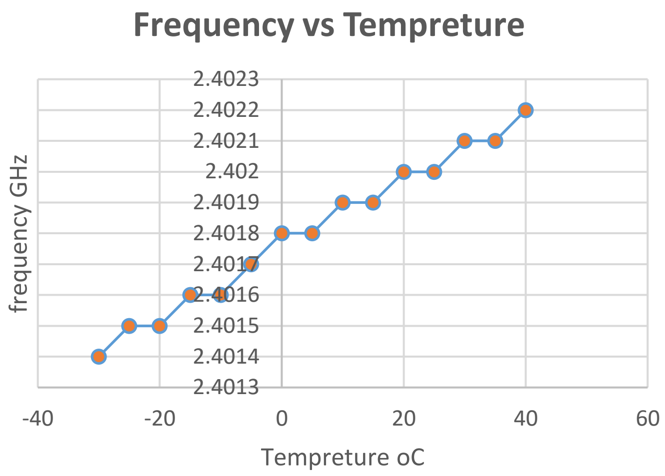
Fig 3.6 Absolute value of the admittance vs. frequency

Also, by using the traditional 3–dB bandwidth method, in which Q (quality factor) at the resonance is calculated by the full width half maximum (FWHM) of admittance.

$$Q_r = \frac{F_r}{\Delta F_r} = 1548$$

3.4.2.3 Study 3: Presressed Analysis, Eigen frequency

Varying the thermal expansion coefficient as a function of temperature (T) to study the effect of the temperature on the resonance frequency and search for the fundamental mode in the Eigen modes shapes. TCF (Temperature coefficient of frequency) which is to b very low ~zero, it is defined as : TCF $= \frac{1}{F_r}\frac{\Delta F}{\Delta T}$, the simulation sweep the temperature between (-30 ^{o}C to 40 ^{o}C) and following graph is obtained.



Which result in a TCF = 4.6 ppm/ ^{o}C

Table 3.3 summarize all the parameter used in Comsol and table 3.4 summarize the results

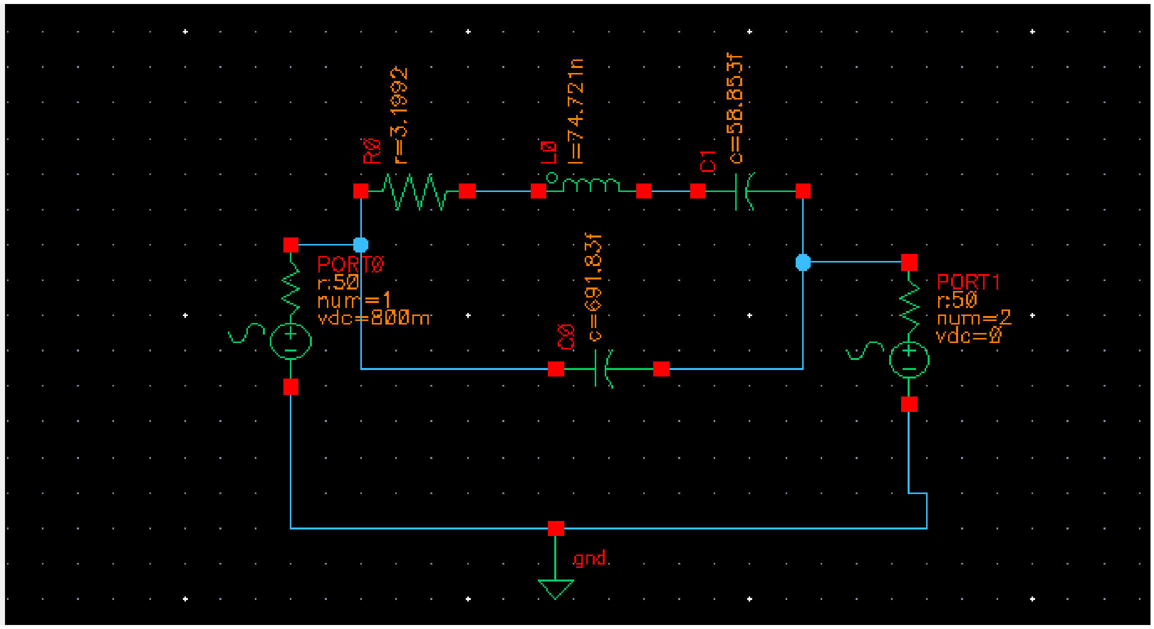
Section	Thickness um	Material
Electrodes	0.115	W
Piezolectric	1.115	AlN

Table 3.3 material geometry

Aspect	Thickness um
Resonance frequency (GHz)	2.4
Quality Factor	1548
TCF 4.6 (ppm/ ^{o}C)	4.6

Table 3.4 aspects obtained from Comsol

3.4 Cadence Simulation



The above circuit is simulated with cadence by running S-parameter study to get the phase depth (the difference between the highest and lowest point on S21 dB curve) and the insertion loss table 3.5 summarize all the aspects

Aspect	**W/AlN/W**	**Si-ware resonator**
Resonance frequency (GHz)	2.4	2.4
Quality Factor	1548	2700
TCF (ppm/ ^{o}C)	4.6	-65
Insertion loss dB	-500 u	10
Phase depth deg	174	120

Table 3.4 aspects obtained from Comsol and Cadence compared with Si-ware asoects

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