Enabling the 5G: Modelling and Design of High Q Film Bulk Acoustic Wave Resonator (FBAR) For High Frequency Applications

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Abstract— ***Micro-electromechanical systems (MEMs) started to dominate the interests of the industry due to the high growth of the various radio frequency (RF) systems, such as mobile telecommunication, satellite communication and other wireless devices that accrues high frequency range. In addition to the race of miniaturizing the device feature size. However, the main obstacle of enabling such devices is that not all of the MEMS technologies are compatible with integrated circuits (IC) manufacturing process. MEMs' devices that are based on acoustics waves like surface acoustic wave (SAW) and bulk acoustic wave (BAW) overcome aforementioned limitations while providing an outstanding performance. BAW resonator is a new technology raised during the last decade which shows better temperature stability compared to SAW, better selectivity, IC manufacturing process compatibility, and lower insertion loss. Filters based on BAWs show very promising results as well. However, BAW resonators still need optimization to achieve the high-quality factor also the temperature dependency is still a big problem. A novel Thin Film bulk acoustic resonator (FBAR) design is presented in this paper using aluminum nitride (AlN) as peizoelectric material and Tungsten (W) for the electrodes, with detailed electrical model and FEM simulations using COMSOL MULTIPHYSICS. In addition, Cadence Virtuoso is used to implement and simulate the electrical model. A resonance frequency of 2.4 GHZ is achieved with quality factor (QF) of 1548 and Temperature coefficient of frequency (TCF) ~ 4.6 (ppm/ oC).***

Keywords—BAW Resonator, Filter, TCF, finite element modeling (FEM), Quality factor, COMSOL MULTIPHYSICS, Cadence.

I. INTRODUCTION

Adding new functionalities to an existing device or material is not the only key to the innovation, nowadays the race to develop the miniaturized devices with high efficiency showing the high importance of integrating new materials into silicon MEMS devices. Moreover, wireless communication systems draw the most interest towards such technologies due to the fast development in IoT applications in fields. However, the main issue is that not all the MEMs manufacturing processes are with integrated circuits (IC) manufacturing process. MEMS devices that use acoustic waves such as SAW and BAW resonators, shown in Fig 1.a and 1.b respectively, overcome the limitation of IC integration compatibility. Besides, the wavelength and the propagation velocity of the electromagnetic wave at certain frequency is directly related to the device size, so as the acoustic waves has about 4 or 5 times less propagation velocity than the electromagnetic waves which leads to a lower device size.

But Why BAW? For frequencies above 2 GHz which is needed in telecommunication technology as well as other wireless applications, SAW resonators can't achieve the requirements of insertion loss, pass-band and power handling control. In addition, SAW resonators are very sensitive to temperature variations, which affects the device QF dramatically. One the other hand, the electrode's stress in BAW is much less than in SAW, which allows the BAW to handle high frequency and power applications with while maintaining high performance.

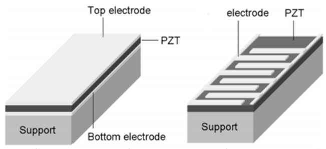

Fig 1 a: Surface Acoustic Wave Resonator. b: Bulk Acoustic Wave Resonator (8)

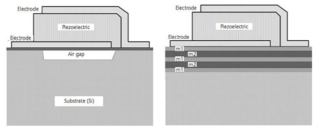

Fig 2 a: film bulk acoustic resonators (FBAR). b: solidly mounted resonators (SMR) (8)

The simplest BAW structure is illustrated in Fig 4, where a piezoelectric material is sandwiched between two metal electrodes, where the lateral energy leakage is the main key for determining the quality factor of BAW and the wave must be confined for the resonance of the device. BAW has two confinement categories as shown in Fig 2, FBAR and solidly mounted resonators (SMR). The driving idea for both is to reduce the losses of the wave into the substrate, for FBAR, the air gab act as a short circuit which forces the wave to reflect only between the two electrodes, as for the SMR the bragg reflector is the confinement method. The only advantage of SMR over FBAR is the better mechanical stability, however FBAR still provides better quality factor. Also the thickness and material of the piezoelectric and electrodes play a very important role in determining the resonance frequency for BAWs. This will be discussed in details in electrical model section. There are several applications in which acoustic resonators can be found such as global positioning systems (GPS, Galileo), data transfer (WLAN, Bluetooth), cellular mobile systems (CDMA, UMTS, GSM), satellite communications and other applications such as military applications [1].

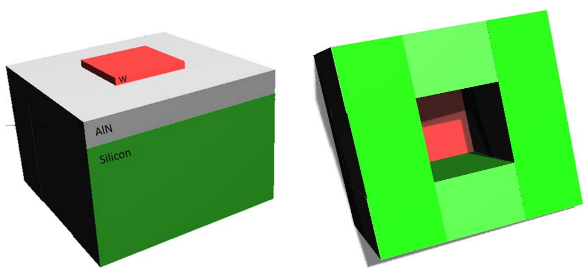

Fig 3 Left: 3D outside view for W/AlN/W design. Right: 3D inside view for the design

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II. PROPOSED BAW RESONATOR MODEL

In this paper, a detailed FBAR resonator design will be presented and simulated with COMSOL and Cadence. The design proposed in this paper, shown in Fig 3, is based on FBAR technology which uses the air gap as a confinement method. Aluminum-nitride (AlN) has been used as a piezoelectric material and Tungsten (W) for the electrodes. The operating frequency of the resonator is 2.4 GHz.

Acoustic wave is excited by an alternating voltage source between the two electrodes which results 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) longitudinal thickness direction and (ii) lateral shear direction. Any lateral wave propagation considered as unwanted mode that affects the quality factor negatively. " QF is a parameter of an oscillatory system or device, such as a laser, expressing the relationship between stored energy and energy dissipation" [2].

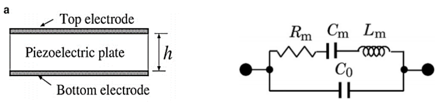

Fig.4 a: Bulk Acoustic Wave Resonator.
b: Electrical equivalent circuit model (BVD model) [3]

A. *Electrical model Design*

The simplest model to model the propagation in a piezoelectric material is a plate with thickness h as in Fig 4, which will have its fundamental resonance frequency *f* when Y (impedance) → 0 at f=(nV)/(2h) (1)

Where V is the acoustic wave velocity, and n is an integer called the order of resonance mode [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 C_0, which means the we can predict the resonance frequency electrically

The simplest known electrical model is the Butterworth–Van Dyke (BVD) circuit model shown in Fig 4 where Cm, Lm, and Rm are the motional capacitance, inductance, and resistance, respectively and C_0 is the clamped capacitance which denotes the electrostatic coupling between two electrodes.

The following the relation reported in [4] that can drive all BVD model as well as the quality factor and Effective coupling coefficient.

$$k^2_{eff}=\frac{\pi^2}{8}\left(\frac{\omega_r^2-\omega_a^2}{\omega_a^2}\right) \quad (2) \qquad Q=\frac{\omega}{2}\cdot\frac{C_mV^2+C_0V^2+L_mI_2^2}{R_mI_2^2+R_0I_1^2} \quad (3)$$

Table 2: Some if the interested piezoelectric materials and crystals properties

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 1. Some if the interested Electrodes materials properties

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

The quality factor can be get by many ways the most traditional one is the 3db-bandwidth. There are many other electrical equivalent models like Mason's Equivalent Circuit Model [4] which are more accurate and take into account the losses in the piezoelectric and the damping loses in general. However, for the sake of simplicity, this work implements the BVD to model the BAW in Cadance.

B. *Material and Thickness*

C.1) Electrodes

The only way to choose the electrodes material is to look into the material acoustic impedance. Choosing material with high acoustic impedance implies that the material can prevent the leakage of the wave outside the active region and efficiently confine the wave. This shall 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, table1 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.

C.2) Piezoelectric materials

Following equation 1, 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 coefficient and compatible with IC manufacturing process. ZnO and AlN coming in the top list of piezoelectric materials that posses all of these properties. Table 2 [5][7] 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), the high longitudinal velocity makes AlN can be used in very high frequency range which is the scope of this work.

To start work with AlN, all the material properties should be determined, 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) [$\times10^{-11}$ F/m]:

$$\begin{bmatrix} 8 & 0 & 0 \\ 0 & 8 & 0 \\ 0 & 0 & 9.5 \end{bmatrix}$$

(ii) Elasticity matrix (stiffness) [×10-11 N/m2] :

$$\begin{pmatrix} 3.45 & 1.25 & 1.2 & 0 & 0 & 0 \\ 1.25 & 3.45 & 1.2 & 0 & 0 & 0 \\ 1.2 & 1.2 & 3.95 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.18 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.18 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.1 \end{pmatrix}$$

(iii) Piezoelectric constant matrix [C/m]:

$$\begin{bmatrix} 0 & 0 & 0 & 0 & -0.48 & 0 \\ 0 & 0 & 0 & -0.48 & 0 & 0 \\ -0.58 & -0.58 & 1.55 & 0 & 0 & 0 \end{bmatrix}$$

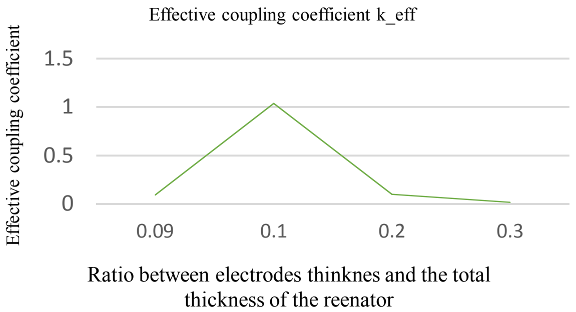

Fig 5 Effective coupling coefficient as a function of electrode thickness for a symmetric membrane AlN resonator.

C.3) Thickness

Putting all together, a stack of W/AlN/W was choesn 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, according to equation 2 it also depend on the thickness of each material used in the device. Fig 5 represents a parametric sweep which was done with different thicknesses to show the effect of the ratio between the thickness of the two W electrodes and the AIN piezoelectric layer on the coupling coefficient.

III. W/ALN/W FBAR RESONATOR DESIGN DIMENSIONS

From equation 2 and for a resonance frequency of 2.4GHz the Effective coupling coefficient can be calculated and from Fig 5 the best ratio between the thickness of the electrodes to the thickness on the piezoelectric is 0.1, Fig 6 clarify all the dimensions used.

IV. FEM SIMULATION (COMSOL)

A full simulation has 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 fundamental resonance mode shape and finally the quality factor.

A. Setting the environment

Start with piezoelectric module, a 3 um PML (perfectly matched layer) is added on the both sides of the design to eliminate any error due 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, 100um is defined as the out-of-

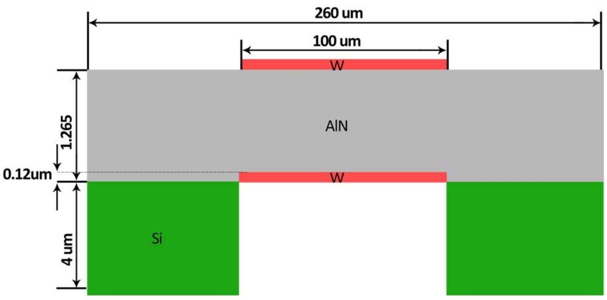

Fig 6 2D model for FBAR W/AlN/W with full geometry details

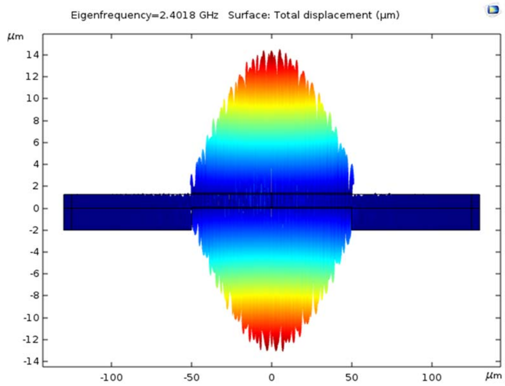

Fig 7 The lowest bulk acoustic mode of the resonator identified from the solutions of the eigenfrequency analysis

plan distance and Finally, parameter T is defined with initial value 300 [K]. The frequency response (Frequency domain study) of the resonator is used to analyze the device within the desired bandwidth of 2 GHz to 3 GHz. A step of 0.01 is used for the eigenfrequency study. Finally, a pre-stressed Eigen frequency study is added with the same setting for the eigenfrequency study to show the response of the design with different temperatures (T).

B. COMSOL Simulation results

The figures are extracted from Mode Shape (solid) which its data set is the eigenfrequency study. And from Displacement (solid) which its data set is the Frequency domain study.

Fig 7 shows the lowest Eigen mode which occurs at 2.4018GHz which is fundamental longitudinal thickness mode and the operation frequency which the peak of the resonance at admittance should match. Also note that COMSOL MULTIPHYSICS computes complex valued eigenfrequencies where the imaginary part gives a measure of the damping due to structural loss, polarization loss and anchor loss here the unwanted mode that has loses around 0.001.

Fig 8 shows the absolute value of admittance as a function of frequency in db. Note that the highest peak in admittance occurs at the lowest BAW mode of 2.4 GHz. Also, by using the traditional 3–dB bandwidth method, in which QF at the resonance is calculated by the full width half maximum (FWHM) of admittance. $Q=f_r/\Delta f_r=1548$.

Resonance frequency (fr) variations against temperature is one of the most important characteristics of acoustic resonators. From such a dependency one can get TCF. To do

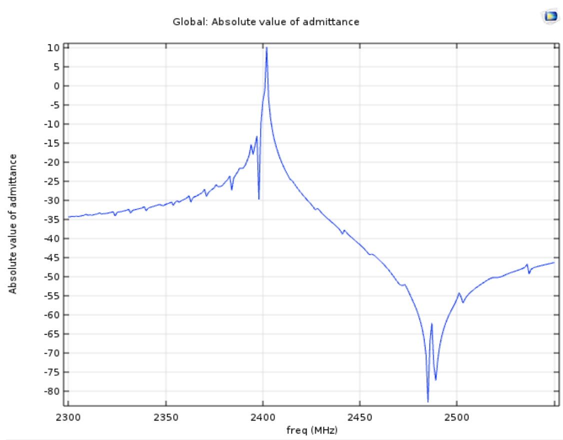

Fig 8 Absolute value of the admittance vs. frequency

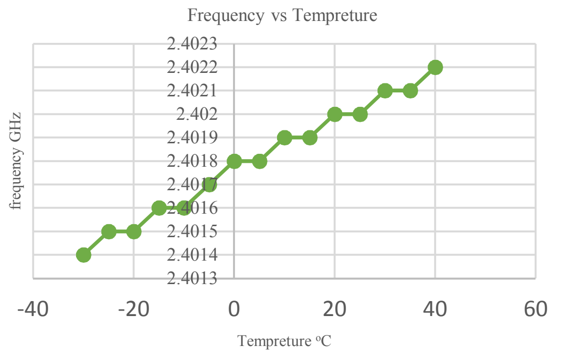

Fig9 Varying the thermal expansion coefficient as a function of temperature (T)

so, we start by varying the temperature of the structure by adding a thermal expansion node while sweeping on T and observe the frequency change against temperature. Another method is to measure the frequency shift according to stress stiffening and temperature dependent Young's modulus. In this paper the first method is used. A low temperature coefficient (TCF) of the resonator is particularly important to guarantee the best phase-noise performance [6]. TCF is defined as follows: TCF = $(1/f_r)*(\Delta F/\Delta T)$. In the simulation setup the temperature is swept in the range (-30 ºC to 40ºC) and the results are shown in Fig 9. The results indicate a TCF of 4.6 ppm/ ºC. Note that in this simulation for TCF, only the temperature variation with the thermal expansion coefficient of the material has been taken into considerations. So, it's expected that this value may change a little when accounting for other factors. Table 3 summarizes the results.

Table 3 results obtained from Comsol and Cadence

Aspect	W/AlN/W
Resonance frequency (GHz)	2.4
Quality Factor	1548
TCF (ppm/ ºC)	4.6
Insertion loss dB	-500 u
Phase depth deg	174

V. CADENCE SIMULATION

Following the modified BVD model and by using the Matlab code all the parameter required for the simulation is obtained. Fig 10 and Fig 11 show the circuit model, which is simulated in cadence by running S-parameter study to get the phase depth (the difference between the highest and lowest point on S21 dB curve). With R_0=3.1992Ω, L_0=74.72n, C_1=58.8531, C_0=691.831and two V_{dc} ports. The obtained Phase depth was 174 deg with insertion loss of about 500 udB. All the results are summarized in table3

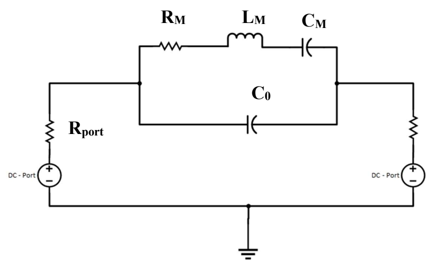

Fig 10 the Cuircut Cadence Modeling

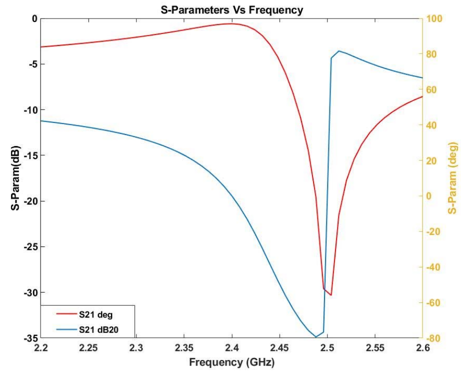

Fig11 Cadence S21 dB curve showed the insertion loss

VI. RECOMMENDATIONS FOR A HIGHER QUALITY FACTOR AND UNWANTED MODES ELIMINATIONS[3][4]

There are several ways to eliminate the unwanted lateral modes which affect negatively the quality factor, from these methods is using (i) Anodized structure, shown in Fig 12.a, which depend on decreasing the area between the two electrodes that can form standing waves, (ii) Thickened edge load, shown in Fig 12.b, which introduces an impedance difference between the air or vacuum and the active region (iii) Step-like frame FBAR, shown in Fig 12.c.

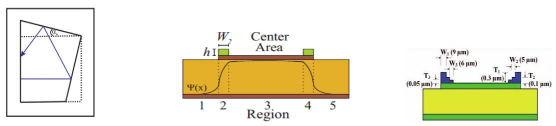

Fig 12 a Anodized b. Thickened Edge Load c. Step-like Frame FBAR

VII. CONCLUSION

, In this paper, the designed FBAR operates at frequency 2.4 GHz. It is successfully designed and simulated using COMSOL simulation and Cadence analysis. The analysis on the effect of electrode thickness, width and length, the material and dimensions of piezoelectric and the quality factor are discussed to show the performance of FBAR. This design is a good candidate as it achieves high Q factors, low TCF and low insertion loss at 2.4 GHz.

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