Research and Design of High Sensitivity FBAR Micro-mass Sensors

Jiatai Ren, Hequn Chu, Yuhui Bai, Rui Wang, Pengguang Chen and Jianming Chen*
Faculty of Science, Kunming University of Science and Technology, Kunming, China
*Corresponding author: jm-chen@kust.edu.cn

Abstract. Micro-mass sensors have important application in chemical and biological sensing. Based on the theory of thin film bulk acoustic resonator (FBAR), this paper represents four designs of different micro-mass sensor models. COMSOL MultiphysicsTM software is used to simulate the FBAR sensor sensitivity, which with low-impedance acoustic layer and additional electrode frame. In the finite element simulation models, five different values of mass-loading were applied. From the experimental results, the characteristic parameters and the sensitivity of the FBAR sensors were obtained. It is known to us that the FBAR sensor’s frequency quality factor can be improved by using the electrode frame, and its sensitivity can be enhanced by using the low-impedance acoustic layer. To sum up, the above analysis shown that the best sensitivity is $1.351 \times 10^{-12} \text{ng/μm}^2/\text{Hz}$ and the frequency quality factor is 1415, which is the FBAR sensor with a single-step electrode frame and a low-impedance acoustic layer.

Keywords: Thin film bulk acoustic resonator (FBAR), Micro-mass sensors, Finite element method (FEM).

1. Introduction
In the radio frequency applications, FBAR and the surface acoustic wave resonator (SAW) has been widely used. Since FBAR has so many advantages such as small size, low insertion loss, low power consumption and high frequency and so on, it is better for super high radio frequency applications than SAW. The resonance frequency of FBAR is above GHz, which is 100 times of the commonly used quartz crystal microbalance sensor (QCM) [1]. The operating principle behind of FBAR-based mass sensors is the so-called mass-loading effect. Thus, the increase of mass-loading on the resonator brings about downshifting of the resonance frequency of it. Follow this conclusion, FBAR can be use for micro-mass sensing, which has attracted the attention of scientists in the chemical and biological sensing field, as previous studies [2, 3] of FBAR have been used as liquid, gas, temperature, and mass sensors.

Aluminum nitride (AIN), zinc oxide (ZnO), and lead zirconium titanate (PZT) has been generally used as the piezoelectric materials in FBAR micro-mass sensors [2, 4-7]. This paper focuses on AIN-based FBAR micro-mass sensors, represents four possible designs of different micro-mass sensor models. The effect of electrode structure and low impedance sensor layer for FBAR sensor has been
studied. FBAR sensor’s mass sensitivity and performance have been simulated in FEM with distributed mass loadings. From the experiments, rapid response and high sensitivity has been shown by FBAR-based micro-mass sensor. It is known to us that FBAR sensors have a broad application prospects in micro-mass sensing field.

2. FBAR Principle and Structure

FBAR is typically a three-layer film structure consisting of the bottom electrode, the piezoelectric layer, and the top electrode sputtered and deposited on a silicon substrate through a bulk micro machining process, as shown in Figure 1. When the alternating current (AC) signal is applied to the piezoelectric materials, the electrical signal is converted into mechanical/acoustic wave and will propagate longitudinally in the FBAR device. This longitudinal acoustic wave propagates along the electric field into the resonator and is subsequently reflected back from the bottom electrode. Acoustic wave propagation is highly sensitive to changes in boundary conditions or small perturbations in the physical properties of the propagation medium, which will cause the phase velocity to shift. Hence FBAR can be used as a mass sensor [8].

![Figure 1. Air gap FBAR structure.](image)

The anti-resonance frequency \( f_a \) is calculated as follows:

\[
f_a = \frac{v}{2h} \tag{1}
\]

Where \( v \) represents the longitudinal acoustic velocity of the piezoelectric material and \( h \) represents the thickness of the piezoelectric film. This formula does not take into account the loading effect of the electrode on the piezoelectric layer, so the actual \( f_a \) value is smaller than the calculated one.

Under the action of piezoelectric effect, the piezoelectric layer are coupled with each other through the piezoelectric strain equation [9]:

\[
D = \varepsilon^T E + dT \tag{2}
\]

\[
S = dE + s^E T \tag{3}
\]

and piezoelectric stress equation [10]:

\[
T = c^E S - eE \tag{4}
\]

\[
D = eS + \varepsilon^E E \tag{5}
\]

The symbols \( D, S, \) and \( T \) represent the dielectric displacement, strain and mechanical stress. Where \( \varepsilon^T \) represents the holding permittivity, \( d \) represents the piezoelectric strain constant, \( s^E \) represents the
short-circuited compliance constant matrix, $c^E$ represents the elastic stiffness matrix of materials under constant electric field, $e^s$ represents the holding dielectric coefficient, and $e$ represents the piezoelectric stress constant matrix.

The internal AlN material properties of COMSOL are as follows:

$$c^E = \begin{bmatrix} 410 & 149 & 99 & 0 & 0 & 0 \\ 149 & 410 & 99 & 0 & 0 & 0 \\ 99 & 99 & 389 & 0 & 0 & 0 \\ 0 & 0 & 0 & 125 & 0 & 0 \\ 0 & 0 & 0 & 0 & 125 & 0 \\ 0 & 0 & 0 & 0 & 0 & 130.5 \end{bmatrix} \text{[GPa]}$$  \hspace{1cm} (6)

$$e = \begin{bmatrix} 0 & 0 & 0 & 0 & -0.48 & 0 \\ 0 & 0 & 0 & -0.48 & 0 & 0 \\ -0.58 & -0.58 & 1.55 & 0 & 0 & 0 \end{bmatrix} \text{[C/m}^2\text{]}$$  \hspace{1cm} (7)

$$e^s = \begin{bmatrix} 9 & 0 & 0 \\ 0 & 9 & 0 \\ 0 & 0 & 9 \end{bmatrix}$$  \hspace{1cm} (8)

Electromechanical coupling coefficient ($k^2_f$) and frequency quality factor (Q) are two parameters that characterize the main performance of FBAR.

$$K^2_f = \frac{\pi^2}{4} \left( \frac{f_a-f_r}{f_a} \right)$$  \hspace{1cm} (9)

The Q factor is defined as the number of cycles in which the entire energy of the structure decreases by an amount of e2π at the resonant or anti-resonant frequencies. The Q factor is calculated as follows

$$Q_{r/a} = \frac{f_{r/a}}{2 \left| \frac{d\angle Z}{df} \right|}$$  \hspace{1cm} (10)

Where $f_r$ is the resonance frequency and $\angle Z$ is the phase response of the input impedance.

3. Sensitivity

The mass load will affect the frequency response of the sensor, reducing $f_r$ and $f_a$, resulting in a frequency shift that is proportional to the mass load. This phenomenon can be described by the Sauerbrey equation[11].

$$\frac{\Delta f_{r/a}}{f_{r/a}} = \frac{\Delta M}{M_0}$$  \hspace{1cm} (11)

In the above equation, $\Delta f_{r/a}$ is the $f_{r/a}$ frequency shift of the sensor with an additional mass load. $M_0$ is the sensor mass; $\Delta M$ is the added mass load to ensure the effectiveness of the device and should be less than 2% of $M_0$.

The ratio of the frequency displacement of the resonant frequency to the mass load is called the mass sensor sensitivity ($S$), as described by the equation:

$$S_{r/a} = \frac{\Delta M}{\Delta f_{r/a}}$$  \hspace{1cm} (12)
4. Model Design
The focus of designing mass sensors is to improve the sensitivity and reliability of the device. A research shows that adding a layer of low-impedance material onto the base of the original structure can lead to the generation of a sensitivity amplification effect [4]. In addition, a frame is attached on the top electrode surface to prevent the leakage of acoustic waves and increase the Q of the device [12].

The methods for the simulation analysis of FBAR devices include the Mason equivalent circuit, the MBVD equivalent model, and and the finite element simulation analysis [10, 13-16]. In this paper, built upon the previous model, FBAR for micro-mass sensing is designed and verified using the COMSOL multiphysics™ finite element simulation software.

In this study, four types of micro-mass sensors are designed with different top electrodes and sensing layers for the pentagonal air gap FBAR with an effective resonant area of 20000μm². As shown in Figure 2. (a) (b) Model #1 employs molybdenum (Mo) for its top and bottom electrodes, each with an effective thickness of 0.2μm, and AlN for the 0.5μm thick piezoelectric layer, while in Model #2 a layer of 0.15 μm thick SiO₂ low impedance acoustic layer material is added to the top electrode of Model #1. Model #3 and #4, as shown in Figure.3, respectively have a single-step electrode frame and a double-step electrode frame attached around the SiO₂ layer of Model #2. Physical parameters used for modeling of FBAR sensors are given in Table 1.

| Materials | Characteristic acoustic impedance (kg/m²s) | Longitudinal wave velocity (m/s) | Poisson's ratio | Young's modulus (Pa) | Density (kg/m³) |
|-----------|------------------------------------------|--------------------------------|----------------|---------------------|----------------|
| AlN       | 3.70e7                                   | 11350                          | --             | --                 | 3300           |
| Mo        | 6.39e7                                   | 6213                           | 0.31           | 3.12e11             | 10200          |
| SiO₂      | 1.25e7                                   | 6253                           | 0.17           | 70e9                | 2200           |

The main purpose of designing these structures in this manner are to improve the sensitivity and Q factor of the micro-mass sensor. Considering the amount of calculations needed for the 3D simulation of the whole device, the model is adjusted to meet the expected design goals before an effective simulation was conducted. In this paper, since the air gap FBAR structure is used, the substrate is neglected in COMSOL modelling [10].

**Figure 2.** Model #1: three-dimensional (a) cross-sectional view (b); Model #2: three-dimensional (c) cross-sectional view (d).
Figure 3. Model #3: three-dimensional (a) cross-sectional view (b); Model #4: three-dimensional (c) cross-sectional view (d).

5. Results and Discussion

5.1. Influence of SiO$_2$ layer and electrode frame structure on resonance characteristics

Figure 4 (a) and (b) are the impedance curves and S11 parameter of the four models when no additional mass load is applied. It can be seen that in the model with the electrode frame, obvious parasitic resonance appears near $f_r$. In all FBAR model simulations, model #1 has the highest $f_r$ and $f_a$, and the largest surface displacement as shown in Figure 5. Table 2 compares the characteristics of these resonators. Models #2, #3, and #4 have the same $f_r$, but the $f_a$ is different, and the impedance values are all increasing. Adding SiO$_2$ layer and electrode frame all reduce the device $f_r$, $f_a$ and $k^2$. The $k^2$ is very important in the filter, because it directly determines the device bandwidth. In the sensor, the frequency quality factor is relatively important, the higher the value, the more stable the device performance. For the thicker electrode area with additional electrode frame, the increase of skin depth makes the effective electrode resistance decrease, resulting in lower ohmic loss, so the $Q_r$ of FBAR with additional electrode frame is higher [17]. At the same time, the electrode frame structure has a better suppression effect on the leakage of shear waves, which makes $Q_a$ increase accordingly. The $Q_a$ of model #3 shows a maximum value of 1415, which is 270 higher than Model #1.

Table 2. Device characteristics without added mass.

| Model | $f_r$ (GHz) | $f_a$ (GHz) | $Q_r$ | $Q_a$ | $k^2$ (%) | Disp (nm) |
|-------|-------------|-------------|-------|-------|------------|-----------|
| #1    | 3.770       | 3.885       | 1252  | 1145  | 7.30       | 2.28      |
| #2    | 3.600       | 3.705       | 1286  | 1151  | 6.99       | 0.56      |
| #3    | 3.600       | 3.690       | 1280  | 1415  | 6.02       | 1.05      |
| #4    | 3.600       | 3.675       | 1290  | 1200  | 5.04       | 0.25      |
5.2. Performance of devices with additional distributed mass

Mass loading is usually achieved by growing or depositing uniformly distributed thin film materials on one electrode of the resonator to cover the active surface of the whole device. Because the FEM software is used in this experiment, we can accurately control the value of mass load through boundary load conditions. Five different values of mass loads were applied to the four models, $0.5 \times 10^{-4}\text{ng/um}^2$, $1.0 \times 10^{-4}\text{ng/um}^2$, $1.5 \times 10^{-4}\text{ng/um}^2$, $2.0 \times 10^{-4}\text{ng/um}^2$, $2.5 \times 10^{-4}\text{ng/um}^2$. The resonant frequency shift of FBAR increases in response to the increase of mass load.

Firstly, Figure 6 (a) shows the results of an analysis performed in terms of $f_r$, where the model with an additional SiO$_2$ layer demonstrating consistent frequency shifts after the same mass load is added, as well as being consistent with its previous performance in the absence of the mass load. All four models show better linear effects when there is an added load mass. Calculation of sensitivity for each model under different mass loads with formula (12) is shown in Table 3. The comparison shows that the sensitivity of the model is more stable when SiO$_2$ layer is added, and sensitivity is higher. Furthermore, as the mass load increases, the sensitivity gradually increases in response.
Next, analyses $f_a$. Figure 6 (b) shows the change of $f_a$, and the linear effect presented is slightly worse than that of Figure 6 (a). Calculate the sensitivity of each model's $f_a$ under different mass loads by formula (12) as shown in Table 4. Model #2 and #3 have the same sensitivity, and when the distributed mass load is $2.5 \times 10^{-4} \text{ng/μm}^2$, the highest sensitivity is $1.351 \times 10^{-14} \text{ng/μm}^2/\text{Hz}$.

Figure 7 (a), (b), (c) and (d) show the displacement of the resonance frequency caused by models #1, #2, #3, and #4 when different mass loads are applied. By comparing the shifting of $f_r$ and $f_a$, it is found that the sensitivity of the model with SiO$_2$ layer is more stable and the sensitivity is higher. The reason is that the top electrode Mo is a kind of high impedance acoustic material, and the attached SiO$_2$ layer is a low impedance acoustic material. They form a pair of Bragg reflectors. Therefore, the acoustic waves can better reach the surface of the sensing layer, thereby increasing the sensitivity. However, the models #3 and #4 with the electrode frame structure have side effects, and there are obvious parasitic resonances near the resonance frequency, as shown in Figure 7 (c) and (d).
Figure 7. Absolute impedance versus shift in resonant frequency plot of models #1, #2, #3, and #4 at different mass loads.

6. Conclusion
In conclusion, we have analyzed four types of FBAR sensors designed with different structures for micro-mass sensing through finite element numerical simulation, determined the influence of low-impedance acoustic layer and additional electrode frame structure on sensor sensitivity. The results show that the additional a single-step electrode frame structure can improve the frequency quality factor of FBAR, as $Q_r$ is increased by 38 and $Q_A$ is increased by 270 compared with the original Model #1. At the same time, there are also some side effects related to the additional frame structure, such as reduced electromechanical coupling coefficient and obvious parasitic resonance. In order to produce high-sensitivity micro-mass sensors, an additional low-impedance acoustic layer attached to the structure can improve the sensitivity of the device, as indicated by the results of Models #2 and #3, where the anti-resonance frequency ($f_\alpha$) shows the highest sensitivity of $1.351 \times 10^{-12}$ng/μm²/Hz.
Acknowledgments
The authors acknowledge the support of Faculty of Science, Kunming University of Science and Technology, for providing the simulation facilities.

References
[1] R.-C. Lin, Y.-C. Chen, W.-T. Chang, C.-C. Cheng, K.-S. Kao, Highly sensitive mass sensor using film bulk acoustic resonator, Sensors and Actuators A: Physical, 147 (2008) 425-9.
[2] L. Garcia-Gancedo, J. Pedros, X.B. Zhao, G.M. Ashley, A.J. Flewitt, W.I. Milne, et al., Dual-mode thin film bulk acoustic wave resonators for parallel sensing of temperature and mass loading, Biosens Bioelectron, 38 (2012) 369-74.
[3] W.R. Ali, M. Prasad, Piezoelectric MEMS based acoustic sensors: A review, Sensors and Actuators A: Physical, 301 (2020).
[4] G. Wingqvist, V. Yantchev, I. Katardjiev, Mass sensitivity of multilayer thin film resonant BAW sensors, Sensors and Actuators A: Physical, 148 (2008) 88-95.
[5] L. Qin, Q.-M. Wang, Mass sensitivity of thin film bulk acoustic resonator sensors based on polarc-axis tilted zinc oxide and aluminum nitride thin film, Journal of Applied Physics, 108 (2010).
[6] H. Campanella, J. Esteve, J. Montserrat, A. Uranga, G. Abadal, N. Barniol, et al., Localized and distributed mass detectors with high sensitivity based on thin-film bulk acoustic resonators, Applied Physics Letters, 89 (2006).
[7] X.L. Zhao, Z.A. Zhao, B. Wang, Z.H. Qian, T.F. Ma, The Design of a Frame-Like ZnO FBAR Sensor for Achieving Uniform Mass Sensitivity Distributions, Sensors-Basel, 20 (2020).
[8] U. Mastromatteo, F.F. Villa, High sensitivity acoustic wave AlN/Si mass detectors arrays for artificial olfactory and biosensing applications: A review, Sensors and Actuators B-Chem, 179 (2013) 319-27.
[9] Zhang, YF; Chen, D, Principle, design and application of thin-film bulk acoustic resonator: Shanghai Jiao Tong University Press; 2011, 28-29. (in Chinese)
[10] R.K. Thalhammer, J.D. Larson, Finite-Element Analysis of Bulk-Acoustic-Wave Devices: A Review of Model Setup and Applications, IEEE Trans Ultrason Ferroelectr Freq Control, 63 (2016) 1624-35.
[11] G. Sauerbrey, Use of vibrating quartz for thin film weighing and microweighing, Z Phys, 155 (1959)
[12] N. Nguyen, A. Johannessen, S. Rooth, U. Hanke, The impact of area on BAW resonator performance and an approach to device miniaturization, Ultrasonics, 94 (2019) 92-101.
[13] F.Z. Bi, B.P. Barber, Improve MBVD model to consider frequency dependent loss for BAW filter design, 2007 Ieee Ultrasonics Symposium Proceedings, Vols 1-6, (2007) 1025-8.
[14] H.H. Guo, A.H. Guo, Y. Gao, T.T. Liu, Influence of external swelling stress on the frequency characteristics of a volatile organic compound (VOC) sensor based on a polymer-coated film bulk acoustic resonator (FBAR), Instrum Sci Technol, 48 (2020) 431-42.
[15] H.P. Wu, X. Cai, Y.L. Wu, Z.G. Lai, Q.H. Yang, W.M. Wang, An Investigation on Extraction of Material Parameters in Longitudinal Mode of FBAR, IEEE T Circuits-Ii, 67 (2020) 1024-8.
[16] C. Muller, M.A. Dubois, Effect of size and shape on the performances of BAW resonators: A model and its applications, 2008 IEEE Ultrasonics Symposium2008, pp. 1552-6.
[17] N. Nguyen, A. Johannessen, U. Hanke, Design of High-Q Thin Film Bulk Acoustic Resonator Using Dual-Mode Reflection, 2014 Ieee International Ultrasonics Symposium (Ius), (2014) 487-90.