Theoretical Simulation and Optimization on Material Parameters of Thin Film Bulk Acoustic Resonator

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1. Introduction

The thin film bulk acoustic resonators (FBARs) are extensively applied for filters, resonators, and sensors, since they were first realized with the resonance frequency of 1.9 GHz in 1999, such as MEMS, biosensors, and gas sensors [1–8]. It is a kind of important device in electronic equipment, and so many kinds of FBARs with high frequency and small dimension have been fabricated during recent ten years for the demand of the industry [9, 10]. The FBARs are especially expected to be investigated and applied by many semiconductor companies such as Agilent, Philip, Murata, and TDK, because of their excellent merits.

Most of researchers focus on the fabrications and the applications of FBAR, and there also are a few researches about numerical simulation and optimization of FBAR. Chao et al. studied the electrode effects of FBAR by Butterworth-van Dyke (BVD) equivalent circuit [11], and Chen and Wang calculated the effective electromechanical coupling coefficient of FBAR [12], and Zhang et al. applied resonant spectrum method to characterize piezoelectric films in FBAR [13]. Besides, our research group published the research about the electrode effect of FBAR [14], and Naumenko analyzed the propagation of acoustic wave in FBAR with Finite Element Method [15], and Kvasov and Tagantsev calculated the nonlinear electrostrictive coefficient with first principles [16]. All of above researches aim at the excellent FBAR performance because the resonance frequency, the effective coupling coefficient, and the accurate optimization for the design of FBAR are the key points for FBAR performance.

As a kind of bulk acoustic resonator (BAR), the figure of merit of an FBAR can be defined by $M = k_{\text{eff}}^2 \cdot Q_S/(1 - k_{\text{eff}}^2)$, and $Q_S$ is the resonance quality factor which is obviously controlled by the piezoelectric layer and electrode effect, and the special research has been done by our research group [14], and so we deeply discuss the material parameter...
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Piezofilm
Top electrode
Bottom electrode

\[ Z_{in} = \frac{1}{\phi H} \begin{bmatrix} 1 & j\omega C_0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \cos \gamma + jZ_E \sin \gamma & Z_0 (Z_E \cos \gamma + jZ_E \sin \gamma) \\ \frac{j \sin \gamma}{Z_0} & 2 (\cos \gamma - 1) + jZ_E \sin \gamma \end{bmatrix}, \]

where \( \phi = k^2 c_0 Z_0 l/V \) is Mason equivalent circuit transfer ratio, \( k^2 \) is the electromechanical coupling factor of piezoelectric film, \( C_0 = \varepsilon_{33} S/l \) is the clamped capacitor with area of \( S \), \( \varepsilon_{33} \) is the dielectric constant with the vertical direction, \( l \) is the thickness of piezoelectric film, \( Z_0 = \rho V S \) is the acoustic impedance of piezoelectric film with the density of \( \rho \), \( V \) is the longitudinal wave velocity, \( \gamma = \omega l/V \) is the phase delay in the piezoelectric film, \( \omega = 2\pi f \) is angular frequency, and \( Z_E \) is the acoustic impedance of electrodes.

We take the electrode material as isotropic, and then we can get the matrix as

\[ \begin{bmatrix} F_1 \\ u_1 \end{bmatrix} = \begin{bmatrix} \cos \gamma_{e1} & jZ_{e1} \sin \gamma_{e1} \\ j \sin \gamma_{e1} & \cos \gamma_{e1} \end{bmatrix} \begin{bmatrix} F'_1 \\ u'_1 \end{bmatrix}, \]

where \( F'_1 \) is zero because of the free top acoustic port, \( \gamma_{e1} = \omega l_{e1}/V_{e1} \) is the phase delay in the top electrode, \( l_{e1} \) is the thickness of top electrode, \( V_{e1} \) is the acoustic velocity of top electrode, \( Z_{e1} = \rho_{e1} V_{e1} S \) is the acoustic impedance of top electrode, and \( \rho_{e1} \) is the density of top electrode.

We can get \( Z_1 \) from (3):

\[ Z_1 = \frac{F_0}{u_0} = jZ_{e1} \tan \gamma_{e1}. \]

Similarly, we can get the acoustic impedance of bottom electrode

\[ Z_2 = \frac{F_2}{u_2} = jZ_{e2} \tan \gamma_{e2}. \]

So the total input acoustic impedance can be given as [13]

\[ Z_{in} = \frac{U}{I} = \frac{1}{j \omega C_0} \left[ 1 - \frac{k^2}{\gamma} \frac{(z_1 + z_2) \cdot \sin \gamma + j \cdot 2 \cdot (1 - \cos \gamma)}{(z_1 + z_2) \cdot \cos \gamma + j \cdot (1 + z_1 \cdot z_2) \cdot \sin \gamma} \right]. \]

Inside (6), \( z_1 = Z_1/Z_0 \), \( z_2 = Z_2/Z_0 \). We take the top electrode and bottom electrode as the same, so the input impedance \( (Z_{in}) \) can be given as (7) with a transfer matrix method [12, 14]

\[ Z_{in} = \frac{1}{j \omega C_0} \left[ 1 - \frac{k^2}{\gamma} \frac{z \sin \gamma + j (1 - \cos \gamma)}{z \cos \gamma + (j/2) (1 + z^2) \sin \gamma} \right]. \]
\[ y = \omega l/V \] is the phase shift in the piezofilm, and \( z = Z/Z_0 \) is the characteristic impedance ratio of the electrodes to the piezofilm as the top and bottom electrodes with the same material and thickness. The series resonance frequency \( f_s \) and the parallel resonance frequency \( f_p \) can be obtained by (7), and then the effective electromechanical coupling factor of FBAR can be demonstrated with the known \( f_s \) and \( f_p \):

\[
k_{\text{eff}}^2 = \left( \frac{f_p^2 - f_s^2}{f_p^2} \right) \equiv 2 \left( \frac{f_p - f_s}{f_p} \right).
\]

Based on the definition published in the IEEE Std. 176-1987 [17], \( f_s \) is the frequency corresponding with the maximum conductance. Then \( f_s \) can be calculated by (7), and \( k_{\text{eff}}^2 \) can be evaluated by (8). However, \( k_{\text{eff}}^2 \) is not only determined by \( k_e^2 \) but also closely related with the electrode and resonator structure.

In the calculation of the resonance frequency \( f_s \) with (7), the dielectric, the piezoelectric, and the elastic constants of the piezoelectric film and the elastic constants of the electrodes generally are complex values, but all others, such as \( k_e^2 \), are considered as real values [12]. In addition, for a given piezofilm, \( C_0 \) is a constant. The complex velocity \( V \) in piezofilms or electrodes was given by a complex expression [12]

\[
V = \left( \frac{C_{33}'' + jC_{33}''}{\rho} \right)^{1/2} \equiv V' \left[ 1 + j \left( \frac{2Q_m}{V''} \right) \right].
\]

\( V' = \sqrt{C_{33}/\rho} \) is the real part, \( V'' = \sqrt{C_{33}'/\rho} \) is the imaginary part, and \( C_{33}'' \) and \( C_{33}' \) are the real part and imaginary part of elastic constant \( C_{33} \), where \( C_{33}' \) is responsible for the mechanical losses, and \( Q_m = C'/C'' \equiv V'/2V'' \) is the mechanical quality factor of the piezofilm or the electrode.

So the resonance frequency and the effective electromechanical coupling coefficient of FBAR can be obtained and analyzed by above definitions and equations.

### 3. Effects of Material Quality Factors on Effective Coupling Factor

The effect of electrode on FBAR performance is studied and shown in the following parts, and the thickness, \( d_e \), the density, \( \rho_e \), and the resonance frequency, \( f_s \), and the effective electromechanical coupling factor, \( k_{\text{eff}}^2 \), are investigated; besides, the acoustic velocity \( v_e \) on \( k_{\text{eff}}^2 \) is also done. The different piezoelectric films of ZnO and AlN with thickness of 2\( \mu \text{m} \) are used in this research, and they both are typical examples in the realistic applications, and the constants of material used in the calculation are shown in Table 1.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density (kg/m^3)</th>
<th>Velocity (m/s)</th>
<th>Impedance ((10^9 \text{ kg/m}^2\text{s}))</th>
<th>(k_e^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnO</td>
<td>5606</td>
<td>6350</td>
<td>35.6</td>
<td>7.50</td>
</tr>
<tr>
<td>AlN</td>
<td>3300</td>
<td>11050</td>
<td>36.5</td>
<td>6.25</td>
</tr>
</tbody>
</table>

The resonance frequency definitions are stated in the IEEE Std. 176-1987 that \( f_s \) is defined as the frequency of maximum conductance [17]. So we can calculate \( f_s \) by setting the conductance maximum with (7). In the calculations, we take the different piezoelectric films with ZnO and AlN and take all other parameters as constants except the density and the thickness of electrode. We can take the different density as different electrode material and study what will happen to the resonance frequency of FBAR if we change the thickness of the same material electrode, which is very valuable for the design of FBAR devices.

The results of \( f_s \) changing with \( \rho_e \) and \( d_e \) of FBAR based on ZnO and AlN piezoelectric films were obtained, and the three-dimensional (3D) figures were shown as Figures 3(a) and 4(a), respectively, and the two-dimensional (2D) figures were shown as Figures 3(b) and 4(b), respectively. It can be obtained that the resonance frequency decreases with the thickness and the density of electrode increasing by the 3D figures, and this rule becomes more typical with the thin electrode or the high density, and it is the most obvious when both thickness and density of electrode appear in large value area. So we can choose proper material with small density and thin electrode for high resonance frequency by these results even though there still are some other parameters which should also be considered such as acoustic velocity. However, if the acoustic velocity in the electrode is a constant, then this result can be effectively used to design and evaluate the resonance frequency according to the application requirement. The above results can also be proved by the two 2D figures. Besides, we also can get that the FBAR decreased over half of resonance frequency just with the thickness change of 0.4\( \mu \text{m} \), and so the thickness effect of electrode on the resonance frequency are very distinct, which becomes smoother in the smaller thickness area.

#### 3.2 Effects of \( \rho_e \) and \( d_e \) on \( k_{\text{eff}}^2 \) of FBAR

Based on the definition published in the IEEE Std. 176-1987 [17], \( f_s \) is the frequency of maximum conductance and \( f_p \) is the frequency of maximum resistance. Then \( f_s \) and \( f_p \) can be calculated by (7), and \( k_{\text{eff}}^2 \) can be evaluated by (8). \( k_{\text{eff}}^2 \) is not only determined by \( k_e^2 \) but also determined by the electrode and resonator structure.

We calculated \( k_{\text{eff}}^2 \) changing with the thickness and the density of electrode, and the 3D figures and 2D figures were given in Figures 5 and 6 with ZnO and AlN piezoelectric films, respectively.

It can be obtained by Figures 5(a) and 6(a) that there is the maximum \( k_{\text{eff}}^2 \) corresponding to some compositions of thickness and density of electrode, which is near the thin electrode and high density area. \( k_{\text{eff}}^2 \) increases and then
Figure 3: $f_s$ of FBAR versus the thickness and the density of electrode with ZnO piezoelectric film.

Figure 4: $f_s$ of FBAR versus the thickness and the density of electrode with AlN piezoelectric film.

Figure 5: $k_{eff}^2$ of FBAR versus the thickness and the density of electrode with ZnO piezoelectric film.
decreases with the thickness increasing, and the increasing ratio can reach to 20% over original value of piezoelectric film. However, $k^2_{\text{eff}}$ mostly increases with the density of electrode. $k^2_{\text{eff}}$ changes fast with the thickness of electrode when the density of electrode is small, and vice versa. The FBAR with the ZnO layer shows that $k^2_{\text{eff}}$ changes more quickly than the case of AlN, and the thickness effect is more obvious too, especially for the small density of electrode cases. Furthermore, we can also get the same witness from the 2D figures of Figures 5(b) and 6(b).

A very interesting result is obtained from 2D figures that $k^2_{\text{eff}}$ will arrive at a maximum area with special thickness values for any density of electrode, and the corresponding thickness area is very obvious at the center, such as the FBAR with ZnO. The thickness beginning with the maximum $k^2_{\text{eff}}$ area is nearly 0.37 μm, and the thickness is nearly 0.5 μm for the AlN case. This is a very interesting and important result, and it means the effect of thickness on $k^2_{\text{eff}}$ has a strong rule which is affected little by the density of electrode material. We analyzed this phenomenon that it is the thickness where standing wave appears, and the difference between these two piezoelectric film cases should be attributed to the different piezoelectric thin films. Moreover, it confirms that the standing wave exists in the FBAR, and the thickness of electrode should be optimized with this merit point, which is effective for all kinds of electrode materials.

3.3. Effects of $v_e$ and $d_e$ on $k^2_{\text{eff}}$ of FBAR. For overall evaluation of $k^2_{\text{eff}}$, the effects of $v_e$ and $d_e$ on $k^2_{\text{eff}}$ were conducted with the 2 μm thick piezoelectric film, and the 2D and 3D figures with four different electrode density choices were given for contrasting. The 3D $k^2_{\text{eff}}$ versus $v_e$ and $d_e$ curves based on ZnO and AlN were shown in Figures 7 and 9, respectively, and the 2D results were shown in Figures 8 and 10 correspondingly. The key parameters and results were marked on the 3D figures. We can get that $k^2_{\text{eff}}$ always rises with the density of electrode for the ZnO case in Figure 7 which also can be observed in above section results, and the maximum $k^2_{\text{eff}}$ always appears at the maximum acoustic velocity during our calculation range. The AlN case is the same behavior as the ZnO FBAR in Figure 9. Moreover, $k^2_{\text{eff}}$ rises more obviously with $v_e$ in the large electrode thickness area and vice versa, and $k^2_{\text{eff}}$ changes little with $v_e$ among the small electrode thickness area and especially least in the high density electrode material area. On the other hand, $k^2_{\text{eff}}$ rises distinctly with the electrode thickness in the low velocity area, but it almost does not change in the high velocity area.
We can conclude that $k_{\text{eff}}^2$ is in the direct proportion to the density $\rho_e$ here, and the acoustic velocity of electrode has a similar effect too, and $k_{\text{eff}}^2$ dominantly rises with $v_e$. The electrode thickness affects small $k_{\text{eff}}^2$ with high $v_e$; moreover, when $v_e$ is high enough, then $k_{\text{eff}}^2$ has almost nothing to do with $d_e$. But $k_{\text{eff}}^2$ changes fast with $d_e$ when $v_e$ is small, and $K_{\text{eff}}^2$ rises with electrode thickness first and then descends with its rising, which was also observed in the former section. The thickness corresponding to the maximum $k_{\text{eff}}^2$ is different with different electrode density; however, it descends with density ascending, which also proves the special value $\rho_e d_e$ corresponding with the maximum $k_{\text{eff}}^2$ of FBAR even though we cannot get this result directly by these figures because there are not so many piezoelectric film parameters considered for proving [14]. All these behaviors are similar for both ZnO and AlN based FBARs.

The density, acoustic velocity, and thickness of electrode of FBAR can be optimized by above results for special $f_s$ and $k_{\text{eff}}^2$ need. We can get the higher $k_{\text{eff}}^2$ with the higher electrode density, and it is also the same to acoustic velocity of electrode material. The best thickness of electrode is decided by density and especially acoustic velocity; however, the thickness effects are obvious when the acoustic velocity is small, but it almost does not change if the acoustic velocity is very big. Moreover, the best thickness corresponding to the maximum $k_{\text{eff}}^2$ is different with different cases, but the values are in the special area comparing with the distinctly variable $v_e$ and $\rho_e$, and it is because we take most of the parameters of piezoelectric thin film as constants, even though these results can be observed in both ZnO and AlN FBARs in this research.

4. Conclusions

In this paper, the following research and results have been given.
(i) Firstly, we derived the input acoustic impedance equation with transfer matrix method, and the simplified impedance equation of FBAR with the same top and bottom electrode is obtained. This equation can be applied extensively to calculate the resonance frequency, the effective electromechanical coupling factor, the mechanical quality factor, and the merit figure of FBAR, which makes the theoretical calculation and optimization easy.

(ii) Secondly, the effect of thickness and density of electrode on the resonance frequency of FBAR was investigated, and it can be obtained that the thickness and the density of electrode affect the resonance frequency obviously, especially at the large thickness and density area. This result shows that the thickness and the material of electrode are very key parameters for the resonance frequency design of FBAR.

(iii) Finally, the effects of thickness, density, and acoustic velocity on the effective electromechanical coupling factor were studied, respectively. The results show that $k_{\text{eff}}^{2}$ is in the direct proportion to both density $\rho_{e}$ and $v_{c}$ of electrode. The electrode thickness affects small $k_{\text{eff}}^{2}$ with high $v_{c}$; moreover, when $v_{c}$ is high enough, then $k_{\text{eff}}^{2}$ has almost nothing to do with $d_{e}$. $k_{\text{eff}}^{2}$ rises with electrode thickness first and then descends with its rising, and the thickness corresponding to the maximum $k_{\text{eff}}^{2}$ is different with different electrode density and $v_{c}$, but they almost locate in the special area.

All above results indicate that the thickness, density, and acoustic velocity of electrode are very important, and they can be applied to optimize and design different kind of FBARs.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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References


