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Effects of aspect ratio on the mode couplings of thin-film bulk acoustic wave resonators

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We studied mode couplings in thin film bulk acoustic wave resonators of a piezoelectric film on a dielectric layer operating with the fundamental thickness-extensional mode. A system of plate equations derived in our previous paper was used which includes the couplings to the unwanted in-plane extension, flexure, fundamental and second-order thickness shear modes. It was shown that the couplings depend strongly on the plate length/thickness ratio. For a relatively clean operating mode with weak couplings to unwanted modes, a series of discrete values of the plate length/thickness ratio should be avoided and these values were determined in the present paper. The results can be of great significance to the design and optimization of film bulk acoustic wave resonators. © 2017 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/). [http://dx.doi.org/10.1063/1.4983890]

I. INTRODUCTION

Acoustic wave resonators made from piezoelectric crystals are key components of electrical circuits called oscillators in a lot of electronic equipment.1,2 As frequency standards, resonators are widely used for time keeping, frequency operation, and signal generation and processing. Frequency shifts in resonators caused by various effects like a temperature change or stress are the foundation of resonator-based acoustic wave sensors. Conventional piezoelectric resonators are made from crystals like quartz and lithium niobate, etc. They may operate with bulk1,2 or surface acoustic waves.3,4 During the last couple of decades, researchers succeeded in depositing with good enough quality a thin piezoelectric film of AlN or ZnO on a silicon layer to form thin-film bulk acoustic wave resonators (FBARs or TFBARs) operating in the GHz frequency range.5–7 FBARs have several advantages over conventional crystal resonators.8,9 They have also been used to make acoustic wave sensors.10,11 Structurally, FBARs are multilayered plates with metal electrodes, a piezoelectric film, and an elastic layer. In this paper we study the most common FBARs in which the c-axis of the piezoelectric films are in the plate thickness direction and the FBARs operate with the fundamental thickness-extensional mode of the plates. There are other structural types of FBARs operating with shear modes12–16 or solidly mounted on an elastic substrate.17,18 Their modeling requires separate and fundamentally different efforts and is out of the scope of the present paper.

Because of the structural complexity and piezoelectric coupling, theoretical modeling of FBARs is very challenging mathematically. Typical theoretical models of FBARs are for the operating thickness-extensional mode only. The simplest models are one-dimensional.14,15,19,20 with onespatial

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variable along the normal direction of the plates only. One-dimensional models are valid for pure thickness-extensional modes which can exist in unbounded plates. With some approximation of the variation of the fields along the plate thickness, Tiersten and Stevens once derived a single two-dimensional scalar differential equation\textsuperscript{21} that can describe the in-plane variation of the operating thickness-extensional mode (transversely varying thickness-extensional mode). The scalar equation has been used in the analysis of a rectangular trapped energy resonator in Refs. 21 and 22, a two-port filter in Refs. 21 and 23, and a rectangular resonator with ring electrodes for sensor application.\textsuperscript{24}

In real applications, in addition to the operating thickness-extensional mode, other modes are often present in the operation of FBARs. These unwanted modes are called spurious modes.\textsuperscript{25} They affect the performance of FBARs and are highly undesirable in general. For a successful device, we need to be able to describe and predict these spurious modes so that they can be avoided through proper design. However, the theoretical models used in Refs. 14, 15, and 19–24 for the thickness-extensional mode alone cannot treat the couplings between the operating mode and the spurious modes. Theoretical modeling of mode couplings in FBARs is crucial to the current design and manufacturing of FBARs.

In our previous paper,\textsuperscript{26} a system of two-dimensional equations for the operating thickness-extensional mode with couplings to the relevant spurious modes was derived. The spurious modes included in Ref. 26 are the in-plane extensional mode, the flexural mode, the fundamental thickness-shear mode, and the second-order thickness-shear mode. These are the modes that are coupled to the operating thickness-extensional mode in the frequency range of interest of FBARs. In Ref. 26, the propagation of these coupled waves in unbounded plates was studied to verify the equations obtained and determine the correction factors in the equations. In this paper we use the equations obtained in Ref. 26 to analyze the couplings between the operating mode and the spurious modes in a finite plate FBAR.

II. GOVERNING EQUATIONS

Consider the four-layer plate in Fig. 1. The $x_2$ axis is determined from $x_3$ and $x_1$ by the right-hand rule. The $x_1$ and $x_3$ axes are in the middle plane of the plate. The total plate thickness is $2h = h'' + h' + h''$. For a free vibration analysis, the electrodes are shorted and the electric field vanishes within the approximation of the plate theory.

We consider straight-crested modes with $u_2 = 0$ and $\partial / \partial x_2 = 0$. The plate theory in Ref. 26 which is to be used in this paper is summarized briefly below. The displacement field is approximated by

$$
\begin{align*}
  u_1 & \equiv u_1^{(0)}(x_1, t) + u_1^{(1)}(x_1, t)x_3 + u_1^{(2)}(x_1, t)x_3^2, \\
  u_3 & \equiv u_3^{(0)}(x_1, t) + u_3^{(1)}(x_1, t)x_3,
\end{align*}
$$

(1)

where $u_1^{(0)}$ is the in-plane extension, $u_1^{(1)}$ is the fundamental thickness shear, $u_1^{(2)}$ is the second-order thickness shear, $u_3^{(0)}$ is the flexure, and $u_3^{(1)}$ is the thickness extension. The relevant plate strains corresponding to Eq. (1) are

\begin{figure}[h]
  \centering
  \includegraphics[width=0.5\textwidth]{fig1.png}
  \caption{A four-layer plate as an FBAR and the defined coordinate system.}
\end{figure}
The resultants in Eq. (3) are related to the plate strains in Eq. (2) through the following plate constitutive relations:

\[
\begin{align*}
S_i^{(0)} &= u_{i1}^{(0)}, \\
S_3^{(0)} &= u_{31}^{(1)}, \\
S_5^{(0)} &= u_{51}^{(1)} + u_1^{(1)}, \\
S_i^{(1)} &= u_{i1}^{(1)}, \\
S_3^{(1)} &= u_{31}^{(1)} + 2u_1^{(2)}, \\
S_5^{(1)} &= u_{51}^{(2)}, \\
T_{11}^{(0)} &= \rho(0)u_1^{(0)} + \rho(1)u_1^{(1)} + \rho(2)u_1^{(2)}, \\
T_{13}^{(0)} &= \rho(0)u_3^{(0)} + \rho(1)k_3u_3^{(1)}, \\
T_{31}^{(1)} - T_{31}^{(0)} &= \rho(1)u_3^{(0)} + \rho(2)u_3^{(1)} + \rho(3)u_3^{(2)}, \\
T_{31}^{(2)} &= \rho(2)u_3^{(0)} + \rho(3)u_3^{(1)} + \rho(4)u_3^{(2)}, \\
T_{11}^{(3)} - 2T_{31}^{(1)} &= \rho(2)u_3^{(0)} + \rho(3)u_3^{(1)} + \rho(4)u_3^{(2)},
\end{align*}
\]

(3)

The equations of motion for \(u_1^{(0)}, u_1^{(1)}, u_3^{(2)}, u_3^{(0)}\) and \(u_3^{(1)}\) are

\[
\rho^{(n)} = \int_{-h}^{h} \rho x^3 dx_3.
\]

(4)

The resultants in Eq. (3) are related to the plate strains in Eq. (2) through the following plate constitutive relations:

\[
\begin{align*}
T_{11}^{(0)} &= c_{11}^{(0)}S_1^{(0)} + k_1c_{13}^{(0)}S_3^{(0)} + c_{11}^{(1)}S_1^{(1)} + c_{11}^{(2)}S_1^{(2)} \\
&+ c_{13}^{(2)}S_1^{(2)} + c_{13}^{(3)}S_1^{(3)} + c_{13}^{(4)}S_1^{(4)} - \frac{c_{44}^{(2)}}{c_{44}^{(4)}} - \frac{c_{44}^{(3)}}{c_{44}^{(4)}}, \\
T_{13}^{(0)} &= c_{11}^{(1)}S_1^{(1)} + \frac{c_{13}^{(1)}}{c_{13}^{(3)}} + c_{11}^{(2)}S_1^{(2)} + c_{11}^{(3)}S_1^{(3)} \\
&+ c_{13}^{(2)}S_1^{(2)} + c_{13}^{(3)}S_1^{(3)} + c_{13}^{(4)}S_1^{(4)} - \frac{c_{44}^{(2)}}{c_{44}^{(4)}} - \frac{c_{44}^{(3)}}{c_{44}^{(4)}}, \\
T_{31}^{(1)} &= \frac{c_{11}^{(1)}}{c_{11}^{(1)}} + k_1c_{13}^{(1)}S_3^{(1)} + c_{11}^{(3)}S_1^{(3)} + c_{11}^{(4)}S_1^{(4)} - \frac{c_{44}^{(2)}}{c_{44}^{(4)}} - \frac{c_{44}^{(3)}}{c_{44}^{(4)}}, \\
T_{33}^{(0)} &= k_1c_{13}^{(0)}S_3^{(0)} + \frac{k_1c_{13}^{(1)}}{c_{13}^{(3)}} + k_1c_{13}^{(2)}S_3^{(2)} + c_{13}^{(3)}S_1^{(3)} \cdot k_1\gamma S_3^{(0)}, \\
&+ k_1c_{13}^{(2)}S_3^{(2)} + c_{13}^{(3)}S_1^{(3)} + c_{13}^{(4)}S_1^{(4)} - \frac{c_{44}^{(2)}}{c_{44}^{(4)}} - \frac{c_{44}^{(3)}}{c_{44}^{(4)}}, \\
T_{11}^{(2)} &= \frac{c_{11}^{(2)}}{c_{11}^{(2)}} + c_{13}^{(2)}S_3^{(2)} + + c_{13}^{(4)}S_1^{(4)} - \frac{c_{44}^{(2)}}{c_{44}^{(4)}} - \frac{c_{44}^{(3)}}{c_{44}^{(4)}}, \\
T_{33}^{(2)} &= k_1c_{13}^{(2)}S_3^{(2)} + \frac{k_1c_{13}^{(2)}}{c_{13}^{(3)}} + k_1c_{13}^{(4)}S_3^{(4)} + c_{13}^{(3)}S_1^{(3)} \cdot k_1\gamma S_3^{(2)},
\end{align*}
\]

(5)

where

\[
C_{pq}^{(n)} = \int_{-h}^{h} c_{pq}x^3 dx_3.
\]

(6)

and \(C_{pq}\) are the usual elastic constants. In Eq. (5), we have denoted
\[\gamma_{3110} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2} \gamma_{3130} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2}\]
\[\gamma_{3111} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2} \gamma_{3112} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2}\]
\[\gamma_{3210} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2} \gamma_{3230} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2}\]
\[\gamma_{3211} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2} \gamma_{3212} = \frac{c_{33}^2 c_{13} - c_{33} c_{13}^2}{c_{33}^2 c_{33} - c_{33} c_{33}^2}\]

\[
\kappa_0, \kappa_1, \kappa_2 \text{ and } \kappa_3 \text{ are correction factors,}^{26} \text{ whose values will be given later. With successive substitutions from Eqs. (2) and (5), we can write Eq. (3) as five equations for } u_1^{(0)}, u_1^{(1)}, u_1^{(2)}, u_3^{(0)} \text{ and } u_3^{(1)}:
\]
\[
\begin{align*}
\begin{pmatrix}
\kappa_0^2 (1) \\
\kappa_1 (1) \\
\kappa_2 (1) \\
\kappa_1 (1) \\
\kappa_2 (1)
\end{pmatrix}
&= u_1^{(0)} + u_1^{(1)} + u_1^{(2)} + 2 u_1^{(3)} \\
&= \rho (0) u_1^{(0)} + \rho (1) u_1^{(1)} + \rho (2) u_1^{(2)} + \rho (3) u_1^{(3)}
\end{align*}
\]
III. FREE VIBRATION SOLUTION OF A FINITE PLATE

where we have introduced the following dimensionless frequency and dimensionless wave number:

\[ \Omega = \omega h \sqrt{\frac{\rho}{c_{44}}}, \quad \xi = kh. \]  

For nontrivial solutions of the wave amplitudes, the determinant of the coefficient matrix of Eq. (15) has to vanish, i.e.,

\[ \det [C(\Omega, \xi)]_{5 \times 5} = 0. \]  

Eq. (17) is a polynomial equation of degree five for \( \xi^2 \). For a given \( \Omega \), there are five roots for \( \xi^2 \) or \( \xi \) because the sign of \( \xi \) does not matter in Eq. (14). Corresponding to each root of \( \xi \), the nontrivial solutions of the amplitudes determine the amplitude ratios which are denoted by

\[ A_0 : B_0 : A_1 : B_1 : A_2 : i = 1 : \beta_0 : \alpha_1 : \beta_1 : \alpha_2, \quad i = 1 \sim 5. \]  

Then the general solution to Eqs. (8)–(12) can be written as
which leads to the following frequency equation:

\[ D(\Omega, a/h)_{5 \times 5} = 0. \]  \tag{20} \]

For nontrivial solutions of \( A_0 \), the determinant of the coefficient matrix of Eq. (20) has to vanish which leads to the following frequency equation:

\[ \det [D(\Omega, a/h)]_{5 \times 5} = 0. \]  \tag{21} \]

Corresponding to each frequency, the nontrivial solutions of Eq. (20) determines the mode.

IV. NUMERICAL RESULTS AND DISCUSSION

As a numerical example, we consider the FBAR in Refs. 21 and 26 whose material constants for the piezoelectric film, the silicon layer, and the electrodes are:

\[
\begin{align*}
    c'_{11} &= 20.97 \times 10^{10} \text{N/m}^2, \\
    c'_{33} &= 21.09 \times 10^{10} \text{N/m}^2, \\
    c'_{13} &= 10.51 \times 10^{10} \text{N/m}^2, \\
    c'_{44} &= 10.51 \times 10^{10} \text{N/m}^2, \\
    \rho' &= 5.68 \times 10^3 \text{kg/m}^3, \\
    \epsilon_{31} &= -0.573 \text{C/m}^2, \\
    \epsilon_{33} &= 1.32 \text{C/m}^2, \\
    \epsilon_{15} &= -0.48 \text{C/m}^2, \\
    \epsilon_{11} &= 8.55 \epsilon_0, \\
    \epsilon_{33} &= 10.2 \epsilon_0, \\
    \epsilon_0 &= 8.854 \times 10^{-12} \text{F/m}, \\
    c''_{11} &= 16.57 \times 10^{10} \text{N/m}^2, \\
    c''_{33} &= c''_{11}, \\
    c''_{13} &= 6.39 \times 10^{10} \text{N/m}^2, \\
    c''_{44} &= 7.956 \times 10^{10} \text{N/m}^2, \\
    \rho'' &= 2.332 \times 10^3 \text{kg/m}^3,
\end{align*}\]

and

\[
\begin{align*}
    c'_{11} &= 18.6 \times 10^{10} \text{N/m}^2, \\
    c'_{33} &= c'_{11}, \\
    c'_{13} &= 15.7 \times 10^{10} \text{N/m}^2, \\
    c'_{44} &= 4.2 \times 10^{10} \text{N/m}^2, \\
    \rho' &= 19.3 \times 10^3 \text{kg/m}^3,
\end{align*}\]

respectively. The geometric parameters are determined by

\[ h' = 15 \mu\text{m}, \ h'' = 5 \mu\text{m}, \ h''' = 0.2 \mu\text{m}, \ R' = \rho' h'/(\rho'' h'') = 0.01. \]  \tag{25} \]

For such an FBAR, the correction factors were determined in Ref. 26 by matching the dispersion relations of the relevant coupled waves calculated from both the plate equations and the three dimensional equations. The detailed procedure can refer to our previous paper. For simplicity, the factor values are directly given here:

\[ \kappa_0 = 1.3116, \ \kappa_1 = 2.2822, \ \kappa_2 = 0.7022, \ \kappa_3 = 1.6936. \]  \tag{26} \]

Fig. 2 shows the dimensionless frequency \( \Omega/\Omega_{\text{TE}} \) versus the plate length/thickness ratio \( a/h \), where \( \Omega_{\text{TE}} \) is the fundamental thickness-extensional frequency of an infinite plate \( (a=\infty) \). For the
FIG. 2. FBAR frequency spectra.

FIG. 3. Essentially thickness-extensional modes: (a) $a/h = 30.36, \frac{\Omega}{\Omega_{TE}} = 1.000836237$; (b) $a/h = 50.30, \frac{\Omega}{\Omega_{TE}} = 1.000309792$; (c) $a/h = 70.28, \frac{\Omega}{\Omega_{TE}} = 1.000157753$. 

FIG. 3. Essentially thickness-extensional modes: (a) $a/h = 30.36, \frac{\Omega}{\Omega_{TE}} = 1.000836237$; (b) $a/h = 50.30, \frac{\Omega}{\Omega_{TE}} = 1.000309792$; (c) $a/h = 70.28, \frac{\Omega}{\Omega_{TE}} = 1.000157753$. 
relatively well-studied quartz resonators, similar figures are called frequency spectra and have been systematically calculated\textsuperscript{29–35} because of their important applications in mode coupling analysis. The curves in Fig. 2 are in fact formed by data points close to each other without really connecting them. Each data point represents the frequency of a mode. Corresponding to a particular value of $a/h$, there are infinitely many modes. A few can be seen in the frequency range shown. As to be shown later in Fig. 3, the flat parts of the curves with $\Omega/\Omega_{TE}$ near 1 represent the operating thickness-extensional modes with weak couplings to the other unwanted modes. When the flat parts begin to bend or seem to intersect with other curves, stronger couplings to other modes begin to occur which is undesirable in device operation and should be avoided. The usefulness of the frequency spectra is that it determines when flat parts of the curves in Fig. 1 bend or end, and thus excludes a discrete series of values of $a/h$.

Fig. 3 shows the plate displacement components according to Eq. (1) at the plate upper surface where $x_3=h$. They are for different values of $a/h$ roughly in the middle of the flat parts of the curves.
in Fig. 2 near $\Omega/\Omega_{TE}=1$. Clearly, the thickness-extensional displacement $u_3^{(1)}$ dominates in these modes and hence they are called the essentially thickness extensional modes. From (a) to (c), as $a/h$ increases, the dominance of $u_3^{(1)}$ becomes stronger. This is because for longer plates the edge effects that cause mode couplings are less influential. Therefore, in device applications, plates with large values of $a/h$ are with less mode couplings and are desirable as long as the requirements on size and weight allow. The frequencies of these modes decrease very slightly as $a/h$ increases, which is as expected because the frequencies of the thickness-extensional mode are essentially determined by the plate thickness $2h$ and depend very weakly on the length $2a$, and therefore larger plates have lower frequencies.

Fig. 4 shows four modes corresponding to the four points on the curves in Fig. 4 (a). Fig. 4 (b) is for point A which is in the middle of the flat part of the curves near $\Omega/\Omega_{TE}=1$. It is an essentially thickness-extensional mode with a dominating $u_3^{(1)}$. Fig. 4 (c) is for point B which is near the end of a flat part in Fig. 4 (a). It is still thickness-extensional although $u_3^{(1)}$ is less dominating compared to Fig. 4 (b). This mode can still be used in devices but it is not as ideal as the mode in Fig. 4 (b). In Fig. 4 (d) which is for point C, no plate displacement component is dominating although the second-order thickness-shear displacement $u_1^{(2)}$ is larger than the other displacements. This mode is simply not useful for devices. The mode in Fig. 4 (e) corresponds to point D in Fig. 4 (a) which is in a flat part of the curves that is not one of those that are very close to $\Omega/\Omega_{TE}=1$. Its displacement $u_3^{(1)}$ is much larger than other displacements. However, $u_3^{(1)}$ has two nodal points (zeros) along the plate. This causes the cancellation of charges on the electrodes produced by the thickness-extensional strain through piezoelectric coupling, and, as a consequence, lowers the capacitance of the resonator which is undesirable. Therefore this mode is not useful in applications.

Fig. 5 shows a few modes with large values of $a/h$. The one in Fig. 5 (b) is a nice essentially thickness-extensional mode with a strongly dominating $u_3^{(1)}$. The two other modes are also essentially thickness-extensional but they correspond to the flat parts of the curves in the frequency spectra at

![Fig. 5](image-url)
higher places. Both of these two modes have nodal points and hence the related charge cancellation as discussed after Fig. 4, and are not very useful in devices.

V. CONCLUSION

In FBARs, the operating thickness-extensional mode is coupled to the in-plane extension, flexure, fundamental and second-order thickness-shear modes. The frequency spectra obtained show that these couplings are sensitive to the plate length/thickness ratio. To avoid strong couplings to unwanted modes, a discrete series of values of the length/thickness ratio need to be avoided in design. The essentially thickness-extensional modes are more pure for plates with larger length/thickness ratios. The plate equations derived in our previous paper are ready to be used and are effective in the modeling of mode couplings in FBARs. They can be used to produce the frequency spectra and predict when the mode coupling is weak or strong.

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