SIMULATION OF SECOND-ORDER EFFECTS IN S BAR AND FBAR

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Abstract - Filters employing thin-film bulk acoustic wave (BAW) resonators are important for radio-frequency (RF) selectivity in mobile communication systems and other wireless applications. Accurate device models are needed for this technology. 1D and 2D analytical electro-acoustic BAW resonator models are described here. Application of these models and also 2.5D electromagnetic simulation to resonators and filters of both the membrane and solidly-mounted types is presented. Many of the observed second-order, as well as first-order effects, are seen to be explained either quantitatively or qualitatively.

I. INTRODUCTION

BAW filters are important for front-end selectivity in current and future mobile communication systems \cite{1-4} and other wireless applications \cite{5-9}. These are based on resonators fabricated using thin-film processes. Their advantages include compatibility with silicon IC technology and wafer-scale packaging techniques, as well as the small size and low material losses normally associated with acoustic wave devices. Different types of thin-film BAW resonators have been reported. Both the membrane-based film BAW resonator (FBAR) and Bragg-reflector based solidly-mounted BAW resonator (S BAR) have been extensively studied \cite{1-20}. (Note that the terminology for the two types is not completely consistent across publications.)

To meet the demanding specifications typical in mobile applications it is important to control as many aspects of performance as possible. Simulation using accurate device models is therefore needed to understand not only first-order behaviour, but also the many second-order effects which can degrade performance. A further use of such models is the prediction of effects, which in themselves do not impinge on performance, but which can be used in conjunction with measurement for diagnostic purposes, e.g. to obtain more accurate material data including layer thicknesses.

A 1D analytical electro-acoustic model \cite{15} in which field variations normal to the surface only are considered, was shown to predict some of the observed effects. The justification for the 1D approximation is that lateral resonator dimensions are typically much larger than layer thicknesses. This electro-acoustic model was also combined with 2.5D electromagnetic (EM) simulation \cite{16} to explain other aspects of both resonator and filter performance. However, there is now a growing interest in the influence of additional acoustic effects, particularly laterally propagating wave-guide modes \cite{10-14,17-20} which cannot be explained by such models. More detailed models have therefore been developed in order to explain these weak but nevertheless significant effects. These include a variety of approximate 2D models \cite{10,14,19,20} in which the solution is still obtained in analytical form, and also 3D numerical models \cite{11,18}. Although the 3D models of the acoustic part of the problem are more general, the analytical 1D and 2D solutions can provide more insight and lend themselves more readily to computer-aided design (CAD). In the following sections the electro-acoustic equations are initially expressed in general 3D form \cite{21}, which is then approximated for thin-film BAW device analysis first to 2D and then 1D. The detailed 1D theory and results of combining it with 2.5D EM analysis for SBAR simulation are then presented. This is followed by the detailed 2D electro-acoustic theory and an example of its application to an FBAR device. Extension of the 2D theory to SBAR structures is then discussed.
II. GOVERNING EQUATIONS

Cross-sections through the layers of the types of BAW resonators considered are shown in Fig. 1. The area of overlap between top and bottom electrodes, which to first-order defines the resonator area, is referred to here as the "internal" region. The area outside this is the "external" region. Physical layout in the plane of the layers is considered later.

Since the behaviour of thin-film BAW devices is governed by both acoustic and EM fields, it is necessary to consider two sets of coupled equations: Newton’s equations and Maxwell’s equations (the latter being particularly important for understanding the effect of interconnect and packaging).

Newton’s equations of motion (in the absence of external forces) are:

$$ T_{ij,j} = \rho^2 u_i / c^2 \quad (i = 1..3) \quad (1) $$

where $T$, $\rho$, $u$ and $t$ are stress, density, particle displacement and time respectively. Tensor notation is used here, with a repeated suffix $j$ in this case indicating summation. Since acoustic wavelength, and therefore FBAR or SBAR size, is much smaller than electromagnetic wavelength, Maxwell’s equations (in the absence of free charge) may be accurately approximated, at least for fields within the resonators themselves, by the quasi-static form:

$$ D_{i,i} = 0 \quad (2) $$

where $D$ is electric flux density. Free charge within the layers is assumed to be zero. Physical layout and package modelling typically require other equations from the full Maxwell set, although further quasi-static approximations are also accurate in this context [22]. Details of the EM theory are beyond the scope of this paper. Models of complete BAW filters are based on separate models for each BAW resonator, together with a package/interconnect model, merged into a single circuit-level model, which is then simulated using circuit analysis. The types of material in which the electro-acoustic fields must be considered, and the constitutive relations between the relevant field variables are [21]:

piezoelectric solid

$$ T_{ij} = c E_{ijkl} S_{kl} - e_{klj} E_k \quad (i,j = 1..3) \quad (3) $$

$$ D_i = e_{ikl} S_{kl} + \varepsilon_{ik} E_k \quad (k = 1..3) \quad (4) $$

dielectric solid:

$$ T_{ij} = c_{ijkl} S_{kl} \quad (i,j = 1..3) $$

$$ D_i = \varepsilon_{ik} E_k \quad (i = 1..3) \quad (4) $$

conducting solid:

$$ T_{ij} = c_{ijkl} \delta_{kl} \quad (i,j = 1..3) $$

$$ D_i = \varepsilon_0 E_i \quad (i = 1..3) \quad (6) $$

free space (air):

$$ S_{ij} = 0.5(u_{ij} + u_{ji}) \quad (i,j = 1..3) \quad (7) $$

$$ E_i = - \phi_i \quad (i = 1..3) \quad (8) $$

where, additionally, $\varepsilon$ is strain, $E, \phi$ are electric field and potential, $cE, c$ are elastic constants, $e$ is piezoelectric constant, and $\varepsilon, \varepsilon_0$ are permittivities. In the following analysis, the piezoelectric material is assumed to be of class 6mm with C-axis in the $x_3$-direction, while all other materials are assumed to be isotropic. 1D and 2D approximations to the resonator modelling problem,
in which fields vary spatially only with $x_3$ in the former, and only with $x_1$ and $x_3$ in the latter, are now considered. With reference to Fig.1, introducing the 2D approximation and replacing tensor with matrix notation [21], the differential equations reduce to:

\[ T_{1,1} + T_{5,3} = \rho^2 u_1 / \alpha^2 \]
\[ T_{5,3} + T_{3,3} = \rho^2 u_3 / \alpha^2 \]  
\[ D_{1,1} + D_{3,3} = 0 \]  
\[ (9) \]
\[ (10) \]

And the constitutive relations reduce to:

piezoelectric solid
\[ T_1 = c E_{11} S_1 + c E_{13} S_3 - e_{31} E_3 \]
\[ T_3 = c E_{31} S_1 + c E_{33} S_3 - e_{33} E_3 \]
\[ T_5 = c E_{44} S_5 - e_{15} E_3 \]
\[ D_1 = e_{15} S_5 + \delta_{11} E_1 \]
\[ D_3 = e_{31} S_1 + e_{33} S_3 + \delta_{33} E_3 \]  
\[ (11) \]

isotropic dielectric or metal:
\[ T_1 = c_{11} S_1 + c_{12} S_3 \]
\[ T_3 = c_{12} S_1 + c_{11} S_3 \]
\[ T_5 = c_{44} S_5 \]
\[ D_1 = e E_1 \]
\[ D_3 = e E_3 \]  
\[ (12) \]
\[ (13) \]

where, additionally:
\[ S_1 = u_{1,1} \]
\[ S_3 = u_{3,3} \]
\[ S_5 = (u_{1,3} + u_{3,1})/2 \]
\[ E_1 = -\phi_1 \]
\[ E_3 = -\phi_3 \]  
\[ (14) \]

To derive the admittance of a single resonator a voltage $V_{in} \exp(j \omega t)$, where $V_{in} = 1$, is assumed to be applied to its top electrode with the bottom electrode grounded. The factor $\exp(j \omega t)$, where $\omega$ is angular frequency, is then common to all field variables, and is omitted from subsequent equations. In the electro-acoustic theory electrical losses within the resonators are assumed to be negligible (although in the EM theory used for modelling layout they are included [22]). The boundary conditions for the 2D resonator model are then:

\[ u_1, u_3, T_3, T_5 \text{ continuous on interfaces between solid layers} \]  
\[ (15) \]
\[ \phi, D_3 \text{ continuous on interfaces between layers in which the electric field is non-zero} \]  
\[ \phi = V_{in} \text{ on bottom surface of top electrode} \]  
\[ (17) \]
\[ \phi = 0 \text{ on top surface of bottom electrode} \]  
\[ (18) \]
\[ T_3, T_5 = 0 \text{ on interfaces between solid layers and free-space} \]  
\[ (19) \]

Edge effects in the small regions where layers are discontinuous (e.g. in the region of the top electrode edges) are assumed to be insignificant. In the 1D approximation, the equations further reduce to:

\[ T_{3,3} = \rho^2 u_3 / \alpha^2 \]  
\[ D_{3,3} = 0 \]  
\[ (21) \]
\[ (22) \]

and the constitutive relations reduce to:

piezoelectric solid
\[ (T_1 = c E_{13} S_3 - e_{31} E_3) \]
\[ T_3 = c E_{33} S_3 - e_{33} E_3 \]
\[ T_5 = -e_{15} E_3 \]  
\[ (23) \]

isotropic dielectric or metal:
\[ (T_1 = c_{12} S_3) \]
\[ T_3 = c_{12} S_1 + c_{11} S_3 \]  
\[ (24) \]

where, additionally:
\[ S_3 = u_{3,3} \]
\[ E_3 = -\phi_3 \]  
\[ (26) \]

where the sub-sets of equations 23 and 24 indicated in brackets are not actually used in the 1D model.

Similarly, the boundary conditions reduce to:

\[ u_3, T_3 \text{ continuous on interfaces between solid layers} \]  
\[ (27) \]
\[ \phi, D_3 \text{ continuous on interfaces between layers in which the electric field is non-zero} \]  
\[ (28) \]
\[ \phi = V_{in} \text{ on bottom surface of top electrode} \]  
\[ (29) \]
\[ \phi = 0 \text{ on top surface of bottom electrode} \]  
\[ (30) \]
\[ T_3 = 0 \text{ on interfaces between solid layers and free-space} \]  
\[ (31) \]
Resonator edge boundary conditions corresponding to equation 20 are ignored. In both models the admittance $Y$ of the resonator, equal to the current in the top electrode for unit applied voltage $V_{in}$, is given by the time derivative of its net free charge $Q$:

$$ Y = j\omega Q = -j\omega \int D_3(x_3 = z_o) \, dx_1 \, dx_2 $$

where $z_o$ is the location of a plane an infinitesimal distance below the bottom surface of the top electrode, and the integral is over the electrode area.

### III. 1D MODEL AND RESULTS

For structures of either type shown in Fig.1 a solution of the following form, where the second superscript $n$ indicates layer index, is initially assumed for the internal region:

- in the piezoelectric layer
  
  \begin{align*}
  u_1 &= 0 \\
  u_3 &= B_2(1D,n) \exp[-j k(1D,n)x_3] \\
  \phi &= B_3(1D,n) \exp[-j k(1D,n)x_3]
  \end{align*}

- in other layers
  
  \begin{align*}
  u_1 &= 0 \\
  u_3 &= B_2(1D,n) \exp[-j k(1D,n)x_3] \\
  \phi &= 0
  \end{align*}

Fields in free-space and all layers in the external regions are assumed to be zero. Substituting equations 33-34 into 21-26 gives solutions for the wave-numbers $k(1D,n)$ in all layers, and the amplitude ratio $B_3/B_2$ in the piezoelectric layer. These solutions are referred to as partial waves. Two solutions are possible in each layer, corresponding to equal and opposite $k(1D,n)$. Indicating partial-wave index by the subscript $p$, a more general solution is then given by a linear sum over the partial waves:

- in all layers
  
  \begin{align*}
  u_3 &= \sum_p B_{2p}(1D,n) \exp[-j k_p(1D,n)x_3] \\
  \phi &= \sum_p B_{3p}(1D,n) \exp[-j k_p(1D,n)x_3]
  \end{align*}

- and in the piezoelectric layer only
  
  \begin{align*}
  \phi &= \sum_p B_{3p}(1D,n) \exp[-j k_p(1D,n)x_3] \\
  &+ B_{33}(1D,n)x_3 + B_{34}(1D,n)
  \end{align*}

where it is readily verified that, in addition to the two partial waves, the last two terms on the RHS of equation 36 are also possible solutions of equation 22. The partial wave amplitudes $B_{ip}(1D,n) (i = 2,3)$ are then found by substituting equations 35-36 into the 1D boundary conditions 27-31. Further substitution into equation 32 gives the solution for resonator admittance. The additional passive equivalent circuit extracted from device layout is described in [16,22].

Firstly a single SBAR plus its interconnect is considered. The internal and external regions have 16 and 14 layers respectively, including an aluminium nitride (AlN) piezoelectric layer and 11 Bragg-reflector layers. The substrate is silicon (Si). Simulation is compared with measurement in Fig.2, which shows $Re(Y)$ over a broad frequency range, with detail near resonance (conductance maximum) and anti-resonance (conductance minimum just above resonance) in the insets. The peaks of the relatively low-frequency ripple above and below resonance correspond to the transmission maxima of the Bragg reflector, and consequent high level of acoustic energy in the Si substrate [16]. These details in the response have been used to determine accurate data for the reflector materials. The high-frequency ripple on the lower side of the resonance is due to reflections from the bottom surface of the substrate. This can be included in the model [15,17], but here the substrate has been assumed to have infinite thickness. However, the high-frequency ripple on the upper side of the resonance cannot be accounted for in the 1D model. This is discussed further in the following sections. The behaviour near resonance is

![Fig. 2: Conductance of SBAR – insets show detail near resonance(top left) and anti-resonance (bottom right): measurement (blue), 1D + EM model (red).](image-url)
accurately predicted, while that near anti-resonance is less well modelled. In addition to the un-explained ripple in the measurement there is also some un-explained loss characterised by a higher measured conductance in the null. However, in many respects the model is accurate.

The treatment of acoustic loss is now considered further. In contrast to the acoustic behaviour, the EM behaviour has features which can only be seen over a broad frequency range. These are accurately modelled as described in [16]. In particular electrical loss due to the finite resistivity of the substrate and finite conductivity of the metal layers is accounted for. Acoustic loss is then included by defining an “effective material quality factor” $Q_m$ equal to the magnitude of the ratio of real to imaginary part of all the elastic constants $c, cE$. Its value is chosen to account for the difference between total measured loss and predicted electrical loss. This does not, of course, explain the actual mechanism for the acoustic loss. In fact it is found that $Q_m$ is strongly frequency-dependent, typically being as high as 6000 near resonance and dropping to around 400 at anti-resonance. This demonstrates that the loss is not in fact a material property, but is almost certainly due to design-dependent acoustic scattering. Thus the combined model allows the electrical and acoustic losses to be distinguished, and shows that the former dominates at resonance while the latter dominates at anti-resonance.

A further illustration is given by the ladder filter illustrated in Fig.3. Its predicted and measured S-parameters are shown in Fig.4. The dip at the centre of the $|S_{21}|$ response was introduced by designing the shunt resonators to have a lower anti-resonance frequency than the resonance of the series resonators. This allows the bandwidth to be broadened and can be compensated by including small series inductors at the ports [16]. To achieve the level of agreement shown $Q_m$ was again calculated for all resonators after electrical loss in the layout had been taken into account. Since the low- and high-frequency pass-band peaks are predominantly associated with anti-resonance of shunt resonators and resonance of series resonators respectively, a relatively low value of shunt resonator $Q_m$ and high value of series resonator $Q_m$ were needed to reproduce the measured response. However, measurement of stand-alone series and shunt resonators showed that there was no significant difference between their losses, again indicating that the loss is actually design-dependent rather than material-dependent. The ripple in the null on the high-frequency side of the pass-band, which is not accounted for by the model, corresponds to the ripple near anti-resonance shown in Fig.2.

Fig. 3: Ladder filter schematic (left) and physical layout (right), with bottom metal layer (magenta) shown superimposed over top (yellow); black dots are locations corresponding to nodes in the extracted equivalent-circuit model of the layout; in the complete circuit model of the filter, resonator models are connected between nodes corresponding to their electrode centres on each of the metal layers, rather than directly to each other as in the schematic.

Fig. 4: S-parameters of SBAR ladder filter; magnitude(top) phase (bottom); measurement (S11 red, S21 blue) simulation (S11 magenta, S21 green).
IV. 2D MODEL AND RESULTS

In order to account correctly for the loss and ripple not explained by either the 1D electro-acoustic model or by EM modelling, the electro-acoustic analysis is being extended to 2D. In the 1D model boundary conditions 27-31 are satisfied, but there is no edge boundary condition corresponding to equation 20. Therefore, there are discontinuities in the 1D solution at electrode edges because all fields are assumed to be zero in the external regions, which is physically unrealistic. In the 2D solution equations 15-19 are satisfied exactly, and equation 20 is approximated by a linear combination of the 1D solution considered as the "source field" and a set of acoustic wave-guide modes propagating and/or decaying in the x_1-direction as the "excited field".

The dispersion relations and mode-shapes of the wave-guide modes are found as follows. Firstly, consider a solution in layer \( n \) of region \( r \) (internal or external) of the form:

in piezoelectric and un-shielded dielectric layers

\[
\begin{align*}
\text{u}_1 &= B_1^{(r,n)} \exp[-j k_0^{(r)} x_1 + k^{(r,n)} x_3] \\
\text{u}_3 &= B_3^{(r,n)} \exp[-j k_0^{(r)} x_1 + k^{(r,n)} x_3] \\
\phi &= B_3^{(r,n)} \exp[-j k_0^{(r)} x_1 + k^{(r,n)} x_3] 
\end{align*}
\]

(37)

in other solid layers including the substrate

\[
\begin{align*}
\text{u}_1 &= B_1^{(r,n)} \exp[-j k_0^{(r)} x_1 + k^{(r,n)} x_3] \\
\text{u}_3 &= B_2^{(r,n)} \exp[-j k_0^{(r)} x_1 + k^{(r,n)} x_3] \\
\phi &= 0 
\end{align*}
\]

(38)

in free-space

\[
\begin{align*}
\text{u}_1 &= 0 \\
\text{u}_3 &= 0 \\
\phi &= B_3^{(r,n)} \exp[-j k_0^{(r)} x_1 + k^{(r,n)} x_3] 
\end{align*}
\]

(39)

where \( k_0^{(r)} \) is the \( x_1 \)-component of wave-number common to all layers. For given \( k_0^{(r)} \) substituting equations 37-39 into 9-10 gives partial-wave solutions, in each layer \( n \), with \( x_3 \)-component of wave-number \( k^{(r,n)} \) and corresponding amplitude ratios \( B_2^{(r,n)}/B_1^{(r,n)} \) and \( B_3^{(r,n)}/B_1^{(r,n)} \). A more general solution, in which summations include all allowed values of partial-wave index \( p \) in each layer, is then:

in piezoelectric and un-shielded dielectric layers

\[
\begin{align*}
\text{u}_1 &= \exp[-j k_0^{(r)} x_1] \sum_p B_{1p}^{(r,n)} \exp[-j k_p^{(r,n)} x_3] \\
\text{u}_3 &= \exp[-j k_0^{(r)} x_1] \sum_p B_{2p}^{(r,n)} \exp[-j k_p^{(r,n)} x_3] \\
\phi &= \exp[-j k_0^{(r)} x_1] \sum_p B_{3p}^{(r,n)} \exp[-j k_p^{(r,n)} x_3] 
\end{align*}
\]

(40)

in other solid layers including the substrate

\[
\begin{align*}
\text{u}_1 &= \exp[-j k_0^{(r)} x_1] \sum_p B_{1p}^{(r,n)} \exp[-j k_p^{(r,n)} x_3] \\
\text{u}_3 &= \exp[-j k_0^{(r)} x_1] \sum_p B_{2p}^{(r,n)} \exp[-j k_p^{(r,n)} x_3] \\
\phi &= 0 
\end{align*}
\]

(41)

and in free-space

\[
\begin{align*}
\text{u}_1 &= 0 \\
\text{u}_3 &= 0 \\
\phi &= \exp[-j k_0^{(r)} x_1] \sum_p B_{3p}^{(r,n)} \exp[-j k_p^{(r,n)} x_3] 
\end{align*}
\]

(42)

The inter-layer boundary conditions for the wave-guide modes are given by equations 15-19 with \( V_{in} \) now equal to zero. This latter condition is imposed because the boundary conditions in the internal region (other than those at its edges) are already satisfied by the 1D component solution, and therefore the fields associated with the additional wave-guide mode solutions must not perturb these on any of the layer interfaces. Assuming the \( x_1 \)-dependence in equations 40-42, it is readily verified that a linear term in \( x_3 \) corresponding to that in equation 36 is not an allowed solution of the 2D differential equations. Also the constant term in equation 36 was added arbitrarily to obtain specific voltages on each of the electrodes. Therefore, the number of inter-layer boundary conditions [15-19] is now one greater than the total number of allowed partial modes in all layers. The final boundary condition is then satisfied by solving for complex \( k_0^{(r)} \). This non-linear problem has an infinite number of discrete solutions \( k_{om}^{(r)} (m = 1,2,...) \) corresponding to the allowed wave-guide modes in each region, each with its characteristic frequency-dependent mode-shape \( u_{1m}^{(r)}(x_3) \), \( u_{3m}^{(r)}(x_3) \), \( \phi_{m}^{(r)}(x_3) \). A real value of \( k_0^{(r)} \) indicates an un-attenuated travelling wave, an imaginary value indicates an evanescent (i.e. decaying) wave, and a complex value indicates a decaying travelling wave. Fig.5 shows the dispersion curves (frequency dependence of wave-number) for seven wave-guide modes in the 5-layer internal region and 3-layer...
Fig. 5: Dispersion of seven Lamb-type wave-guide modes in internal region (top) and external region (bottom) of an AlN FBAR; [the blue curve below \( \approx 1.83 \) GHz (internal region), the yellow curve (external region), and the black curve (both regions) are hiding other curves corresponding to complex conjugate solutions.]

The form of these dispersion curves, at least where \( \Omega \) is real-valued, has been confirmed experimentally using an imaging technique [13]. Fig. 6 shows the frequency-dependence of the mode-shape of the internal-region mode corresponding to the red dispersion curve in Fig.5 (top). At 2 GHz this mode is a pure longitudinal wave \( (u_1=0) \) equivalent to the 1D solution, while at \( \approx 2.12 \) GHz it is a pure shear wave \( (u_3=0) \). Both longitudinal and shear components of motion are present at other frequencies. Fig.7 shows the mode-shapes of the other six internal-region wave-guide modes. These are not significantly frequency-dependent near resonance. This is also the case for all seven modes in the external region near resonance (mode-shapes not shown).

Fig. 6: Mode-shape of the internal region Lamb-type wave-guide mode of FBAR corresponding to red dispersion curve in Fig.5 (top); \( x_3 \) is plotted on the horizontal axis with vertical lines indicating layer boundaries; \( |u_1| \) (green), \( |u_3| \) (red); 1.95 GHz (top left), 2 GHz (top right), 2.05 GHz (bottom left) and 2.12 GHz (bottom right).

A general solution for the acoustic field is given by,

\[
\begin{align*}
    u_1 &= \sum_m A_m(r) \exp[-j k_{0m}(r)n x_1] \times \\
         &= \sum_p B_{1p}(r,n) \exp[-j k_{1p}(r,n) x_3] \}
\end{align*}
\]

\[
\begin{align*}
    u_3 &= \sum_p B_{2p}(1D,n) \exp[-j k_{1p}(1D,n) x_3] \\
         &+ \sum_m A_m(r) \exp[-j k_{0m}(r,n) x_1] \times \\
         &= \sum_p B_{2pm}(r,n) \exp[-j k_{pm}(r,n) x_3] \}
\end{align*}
\]
Fig. 7: Mode shapes of six \textbf{internal} region Lamb-type wave-guide modes of FBAR at resonance (2 GHz); correspondence with colours in Fig.5 (top) is: blue (top left), green (top right), yellow (middle left), magenta (middle right), black and its complex conjugate (bottom left and right).

where the $A_m(r)$ are the complex wave-guide mode amplitudes in region $r$, and the first term on the RHS of equation 44 (identical to the 1D solution in equation 35) applies to the internal region only. The edge behaviour of the electric field variable $\phi$ for which the energy is small compared to that in the acoustic field, is ignored. It would require an infinite number of wave-guide modes in each region to satisfy equation 20 for all $x$. However, an approximate solution for the $A_m(r)$ is obtained by satisfying these edge boundary conditions only for a defined set of “principal field components” $\Psi_j(x_j)$ and their gradients $\partial \Psi_j/\partial x_j$ ($j = 1...N_M$). The $\Psi_j$ are obtained by spatially Fourier transforming the solutions for $u_1$ and $u_3$ in equations 43-44 over $x$. For a unique solution the number of “principle field components” must equal the number of wave-guide modes and gradients. Note that, for the internal region, both positive and negative propagating (or decaying) modes are included, whereas for each external region only one of these is allowed since energy must propagate or decay away from the resonator. The accuracy of the solution depends on the choice and number of wave-guide modes and “principle field components”, detailed discussion of which is beyond the scope of this paper. Results are presented for a 100 $\mu$m wide FBAR with all seven modes described above included in the solution. The set of “principle field components” chosen here comprises a three-term expansion for $u_1$ and a two-term expansion for $u_3$ in the piezoelectric layer, and single-term expansions (i.e. mean values) for $u_1$ and $u_3$ in the bottom electrode layer.

The admittance is again given by equation 32, but now calculated from the 2D solution. It therefore includes contributions from the electric displacement coupled to each wave-guide mode term in addition to the contribution from the 1D term. Fig.8 shows (on a log scale) the magnitude of admittance computed using both 1D and 2D models. The 1D solution shows a single resonance at 2 GHz and antiresonance at $\approx 2.048$ GHz. However, the 2D solution also includes weaker resonances due to standing wave-guide modes superimposed on this response at intervals of a few MHz. The contributions to the magnitude of admittance from the 1D component and each of the wave-guide modes are shown in Fig.9. The 1D contribution is seen to dominate (except near resonances), while with reference to Fig.5 the mode

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig8}
\caption{Magnitude of admittance $|Y|$ of 100 $\mu$m wide FBAR predicted by 1D model (blue), 2D model (red).}
\end{figure}
corresponding to the red curve (mode-shape shown in Fig.6), the yellow curve (mode-shape shown middle-left in Fig.7) and blue curve (mode-shape shown top-left in Fig.7) are the next most significant, in that order. Comparing the repeat frequency of the spurious resonances in Figs. 8 and 9 with the wave-numbers in Fig.5, it is clear that the set of standing waves created by reflection from the resonator edges of the yellow mode is the primary cause. It can also be seen from Fig.9 that at each of these weak resonances there is an increase in the amplitude of the red mode. The large individual contributions due to the blue mode and its complex conjugate (hidden) below \( \gamma = 1.83 \) GHz cancel each other and produce no net contribution.

To reinforce the above conclusions two of the “principal field components” (in this case the mean values of \( u_1 \) and \( u_3 \) in the bottom electrode) are shown as functions of \( x_1 \) at the fundamental resonance frequency (2 GHz) in Fig.10, and at one of the spurious resonance frequencies (2.172 GHz) in Fig.11. At the fundamental the red wave-guide mode contribution substantially cancels the 1D source field contribution. At the spurious resonance the standing-wave contributions from the red wave-guide mode (long wavelength) and yellow wave-guide mode (short wavelength) are apparent. The acoustic energy escaping into the external regions in the form of travelling waves can also be seen at both frequencies. Fig.12 shows the solutions at 2 GHz for \( u_1(x_1) \) and \( u_3(x_1) \) in planes just to the left and right of the edge at \( x_1 = W/2 (= 50 \mu m) \). To a good approximation, these components of particle displacement are seen to be continuous across region boundaries, within the continuous layers. Plots of “principal field components”, such as those in Figs. 10 and 11, also demonstrate the required continuity at these boundaries.

Although this simulation is specifically for an FBAR, the mechanism responsible for the spurious resonances is also likely to account for the ripple seen in SBAR measurements such as that in Fig.2. Some 2D models, such as those described in [19-20], include only one wave-guide mode, and therefore do not predict all of the effects discussed here.
Finally SBAR structures are considered. At present the issues of how many and which particular wave-guide modes, and also which "principal field components" should be included, is still under investigation. Nevertheless, much information can be obtained from the behaviour of the wave-guide modes supported by such structures. Fig. 13 shows the dispersion curves for an SBAR with respectively 16 and 14 layers in the internal and external regions, and 11 Bragg-reflector layers. The layers above the reflector are identical to those used in the FBAR analysis. Very broadly the four internal-region SBAR dispersion curves shown correspond to the four FBAR modes with dispersion curves of the same colour in Fig. 5 (top), although in this case the modes are in general Rayleigh-type waves rather than Lamb-type waves.

It may be reasonable to assume that equivalent modes play similar roles in SBAR and FBAR behaviour, although this has yet to be established. There will also certainly be important differences. In particular it can be seen that the internal region red wave-guide mode has zero wave-number at the fundamental resonance frequency of 2 GHz, as in the FBAR case, but complex wave-number at all other frequencies. The mode-shape corresponding to the red curve in Fig.13 (top) is plotted at four frequencies in Fig.14. From these it can be seen that the non-zero imaginary part of wave-number at frequencies away from resonance arises from leakage through the reflector of energy associated with the shear component $u_1$. A similar conclusion was arrived at in [20]. Near resonance the other wave-guide modes are non-leaky surface waves, although the mode corresponding to the blue curve is leaky below $\approx 1.8$ GHz. Their mode-shapes at 2 GHz are shown in Fig. 15. The fact that the red wave-guide mode is both leaky at all frequencies except cut-off and, by analogy with FBAR analysis, also the dominant wave-guide mode, suggests that this may well be the explanation for the much higher values of measured "equivalent material quality factor" $Q_m$ at resonance when compared to anti-resonance, as discussed in Section III. Further it may be reasonable to conclude that the ripple near anti-resonance shown in Fig.2 is due to standing waves of the surface mode with the yellow dispersion curve in Fig.13 (top), with
Fig. 14: Mode-shape of internal region wave-guide mode of SBAR corresponding to red curve in Fig.13 (top); $x_3$ is plotted on the horizontal axis with vertical lines indicating layer boundaries; $|u_1|$ (green), $|u_3|$ (red); 1.95 GHz (top left), 2 GHz (top right), 2.05 GHz (bottom left) and 2.12 GHz (bottom right).

Fig. 15: Mode-shapes of three SBAR internal region Rayleigh-type wave-guide modes at the resonance frequency (2 GHz); correspondence with colours in dispersion curves in Fig.13 (top) is: blue (top left), green (top right), yellow (bottom left).

Mode-shape shown in the bottom left plot in Fig.15. Measured ripple frequency in several devices was close to what would be expected from its computed wave-number and phase velocity [17]. The lower quality factor (compared to FBAR predictions) of the spurious resonances responsible for the ripple near anti-resonance in the SBAR measurement in Fig.2 is probably due to the damping effect of the leaky red wave-guide mode. This appears to be an important difference between FBARs and SBARs. Dispersion curves for the external region of the SBAR are shown in Fig.13 (bottom). The corresponding mode-shapes (not shown) confirm that near resonance all of these are non-leaky surface waves, although the modes corresponding to the red and blue dispersion curves become leaky above $\approx 2.2$ GHz (and are complex conjugates below this).

V. CONCLUSIONS

The electro-acoustic theory of two thin-film BAW resonator models, and the results of applying these models and EM analysis to typical devices have been presented. Many first-order and second-order effects observed in practice are explained by these models. Due to the much shorter wavelengths involved, acoustic effects are more strongly frequency-dependent than EM effects, so the two are clearly distinguishable. Electrical loss in SBARs dominates at resonance where acoustic loss is very low, while acoustic loss dominates at anti-resonance. Probably the most significant second-order effect in thin-film BAW devices is the excitation of unwanted acoustic modes. The 2D model described showed that these are Lamb-type modes in FBARs and Rayleigh-type modes in SBARs. In both cases these are the result of acoustic scattering at physical discontinuities, typically the edges of metalisation patterns. Inclusion of more than one of these modes is necessary to understand some aspects of device behaviour. Although the 2D model is, at present, more applicable to FBARs, indications from predicted dispersion curves (backed up by measurement) are that SBARs exhibit an additional loss mechanism which increases the complexity of its behaviour. Since the Bragg-reflector is optimized only for a normal-incidence extensional wave, other modes such as shear waves are likely to leak energy into the substrate. This is both a disadvantage, because filter insertion loss will increase, and also an advantage because pass-band ripple will be reduced. More work is needed to develop the model to fully characterize this effect. Further extensions, e.g. for modelling filters, based on lateral acoustic coupling of resonators, can be envisaged.
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VII. REFERENCES

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