Abstract: A quantitative analysis tool has been developed which determines the acceleration induced frequency change for surface acoustic waves (SAW) traveling in an arbitrary piezoelectric crystal resonator. This analysis tool uses a finite element approach to solve the static bias problem and Sinha & Tiersten's analytical technique to determine the SAW mode shape. Combining this data with the spatially varying effective elastic constants, the numerical perturbation integral derived by Tiersten determines the acceleration sensitivity of the SAW resonator. The unique aspect of this software is the determination of the spatially varying effective elastic constants using finite element shape functions. The versatility of the tool will be demonstrated by modeling three mounting structures that have been experimentally verified. These mounting structures include two plane stress problems and a plane strain problem.

Introduction

The current emphasis on minimizing development time by incorporating the principles of the system engineering process and concurrent engineering has lead to increased use of computer aided design (CAD) and computer aided analysis (CAA) tools to achieve first run design success. In the field of acoustics, especially when surface acoustic wave devices are considered, many CAD and CAA tools have been developed to aid the engineer in simulating proposed designs. These tools allow the designer to go from a set of design requirements for a SAW device to both a physical layout of the device and a prediction of expected device performance [1-3]. Theoretical device performance calculations use the physical dimensioning of the device combined with the material constants of the piezoelectric substrate to generate the expected device performance data. These analysis tools provide excellent simulations of device characteristics such as quality factor, input and output impedance, and frequency versus amplitude response.

Most of these critical design criteria are well understood for SAW. However, there are many specified requirements for systems that contain acoustic devices which are not well understood and result in iterative engineering solutions where several prototype devices are fabricated for evaluation. Some of these effects include processing, meteorology (temperature, pressure, humidity), residual noise, aging, force, and vibration. Although all of these effects are intriguing and warrant investigation, this paper focuses primarily on the effects of vibration and mode shape on the output frequency of a SAW resonator.

The solution algorithm that was selected to solve the acceleration sensitivity of a SAW device on an arbitrary piezoelectric substrate has four key elements. First, the substrate is parameterized and a finite element mesh of the physical problem is generated. Next, the forces are applied to the finite element mesh and the nodal displacements are calculated forming the solution of the static biasing problem. The material constants and physical characteristics of the SAW device are then used in Sinha and Tiersten's analytical technique to determine the mode shape of the generated SAW. Finally, the mode shape and the spatially varying effective elastic constants determined by the static bias are employed in Tiersten's perturbation integral, and the acceleration sensitivity of the SAW device is evaluated numerically.

The versatility and power of this tool has been verified by using this algorithm to model three examples from the literature [4,5,6]. Good agreement was observed between the results presented in the references and those obtained using this CAA tool.

Acceleration Sensitivity Algorithm

Solution of The Biasing State

The development of the static finite element equations for the solution of the biasing state begins with the general three dimensional equations of elasticity.
\[ T_{ij,t} + \rho b_j = 0, \]  
\[ s_{ij} = \frac{1}{2} (w_{i,j} + w_{j,i}), \]  
and  
\[ T_{ij} = c_{ijkl} \varepsilon_{kl}, \]  
where \( T_{ij} \) are the components of the stress tensor, \( b_j \) are the components of body force per unit volume, \( s_{ij} \) are the components of the infinitesimal strain tensor with \( w_i \) representing the components of displacement, \( c_{ijkl} \) are the components of the 2\textsuperscript{nd} order elastic constants, and \( \rho \) is the mass density of the material. The variational form, or weak form, of equations (1) - (3) is formulated for a body occupying a volume \( V \) bounded by a surface \( S \) as
\[ \delta \Pi = \int_V T_{ij} \delta s_{ij} dV - \int_V b_j \delta w_j dV - \int_S \delta w_j dS = 0 \]  
(4)

The finite element discretization process is applied by interpolating the displacements with a set of shape functions, \( N^q \) as follows:
\[ w_j = N^q w_j^q \]  
(5)
where \( w_j^q \) are the nodal displacements. In equation (5) the superscripts are intended to imply a sum over nodes within an element or an entire mesh, depending upon context. This notation will be employed throughout to save space. The shape functions \( N^q \) may take on several forms and will not be explicitly defined here. The reader is referred to [7] and [8] for these and other omitted finite element definitions. Using equation (5) in the functional (4) gives
\[ \delta \Pi = \left[ \int_{\Omega} \frac{\partial N^p}{\partial x_i} c_{ijkl} \frac{\partial N^q}{\partial x_l} d\Omega w_j^q + \int_{\Gamma} b_j N^p d\Gamma - \int_{\Gamma} t_j N^p d\Gamma \right] \delta w_j^q = 0 \]  
(6)
Here \( \Omega \) represents the discretized domain. For arbitrary variations \( \delta w_j^q \) equation (6) reduces to
\[ K_{jk}^{pq} w_j^q - F_j^p = 0 \]  
(7)
with the elemental equation:
\[ K_{jk}^{pq} = c_{ijkl} G_{lj}^{pq} \]  
(8)
where \( K_{jk}^{pq} \) and \( F_j^p \) are the global stiffness matrix and load vector, with \( k_{jk}^{pq} \) and \( f_j^p \) the corresponding element or local quantities, and
\[ G_{lj}^{pq} = \int_{\Omega} \frac{\partial N^p}{\partial x_i} \frac{\partial N^q}{\partial x_l} d\Omega \]  
(9)
and
\[ F_j^p = \int_{\Omega} b_j N^p d\Omega + \int_{\Gamma} t_j N^p d\Gamma \]  
(10)
Here \( \Omega \) represents the a single element domain with bounding surface \( \Gamma \). The global system is assembled in the usual way giving rise to the matrix problem
\[ K \mathbf{w} = F \]  
(11)
with solution
\[ \mathbf{w} = K^{-1} \mathbf{F}. \]  
(12)

Calculation of the SAW Mode Shape

The general three dimensional surface acoustic wave mode shape is obtained from the straight crested solution obtained by Sinha and Tiersten [11,12,13]
\[ \hat{\alpha}(x_2) = \sum_{n=1}^{4} C^{(n)} A^{(n)} e^{-\beta_n \xi x_2} \]  
(13)
where \( C^{(n)} \) and \( A^{(n)} \) are amplitude ratios, \( \beta_n \) are the decay constants along the \( x_2 \) direction, and \( \xi \) is the straight crested propagation number along the \( x_1 \) direction. With this solution, the transformed variably crested solution is obtained by replacing \( \xi \) with a modified wave number, \( \zeta \), such that
\[ \zeta = \sqrt{\kappa^2 + \xi^2} \]  
(14)
where \( \kappa \) is the approximate wave number along \( x_3 \) for the \( m \)\textsuperscript{th} transverse mode given by
\[ \kappa = \frac{m \pi}{2w} \]  
(15)
with \( 2w \) denoting the width of a strip. With this
transformed variably crested solution, the acoustic field,
\( u_j(x_1, x_2, x_3) \), in the transmission path can be written as a purely real function as

\[
  u_j(x_1, x_2, x_3) = f(x_3) \sum_{n=1}^{4} [A_j^{(n)} \cos(\xi x_1) + B_j^{(n)} \sin(\xi x_1)] e^{-\nu x_2}
\]

where \( A_j^{(n)} \) and \( B_j^{(n)} \) are functions of \( C^{(n)} \) and \( A_j^{(n)} \), \( \nu_n = \beta_n \xi \), and \( f(x_3) \) is defined for odd and even harmonics as

\[
  f(x_3) = \begin{cases} 
  \cos(\kappa x_3) & n = 0, 2, 4, \ldots \\
  \sin(\kappa x_3) & n = 1, 3, 5, \ldots 
\end{cases}
\]

The general solution in the reflector arrays is obtained by solving the approximate two dimensional surface wave equations obtained from the variational formulation of Sinha and Tiersten [11,12,13] and using the resulting transmission matrix in the difference equation solution by Tiersten, et al., [14] to obtain the effective decay constants along \( x_1 \). Using this, the surface wave solution in the reflector arrays may be written as a purely real function of the form

\[
  u_j(x_1, x_2, x_3) = f(x_3) \sum_{n=1}^{4} \left( \tilde{A}_j^{(n)} e^{-\alpha_1 x_1} + \tilde{C}_j^{(n)} e^{-\alpha_2 x_1} \right) \cos \xi x_1
\]

where \( \alpha_1 \) and \( \alpha_2 \) are decay constants, \( \tilde{A}_j^{(n)} \), \( \tilde{B}_j^{(n)} \), \( \tilde{C}_j^{(n)} \), and \( \tilde{D}_j^{(n)} \) are constants related to \( A_j^{(n)} \) and \( B_j^{(n)} \), as well as scale factors derived from the difference equation solutions [12]. The variable \( x_1' \) is simply a translated \( x_1 \) for each reflector array. The normalized mode shape is then obtained as

\[
  g_j^h = u_j / N
\]

where \( N \) is a normalizing constant given as

\[
  N^2 = \int \rho u_j u_j dV 
\]

The amplitude envelopes of the first three transverse harmonics of a typical surface wave mode are plotted in Figures 1 through 3.

### Calculation of the Frequency Shift

The frequency shift under a given static biasing state is computed using Tiersten’s perturbation method [10] for small fields superposed on a bias [9]. The change in resonant frequency of the \( \mu^{th} \) eigen-mode is given as

\[
  \Delta \mu = H_{\mu} / 2 \omega_{\mu},
\]

where

\[
  H_{\mu} = -\int \tilde{c}_{LM} e_i^\mu e_i^\mu e_i^\mu dV
\]

and

\[
  \tilde{c}_{LM} = T_{LM}^i \delta_{\gamma i} + c_{LM} E_{AB}^1 + c_{LM} w_{\mu,i} + c_{LM} \gamma_{\mu,i}
\]

The components \( \tilde{c}_{LM} \) are spatially varying effective elastic constants derived from the biasing state with \( T_{LM}^i \) the biasing stresses, \( E_{AB}^1 \) the biasing strains, and \( w_{\mu,i} \) the biasing deformation gradients. The constants \( c_{LM} \) denote the third order elastic constants for the material.

The perturbation integral (22) is evaluated as a sum over \( N \) elements as

\[
  H_{\mu} = -\sum_{i=1}^{N} \int \tilde{c}_{LM} e_i^\mu e_i^\mu e_i^\mu dV_i
\]

where \( V_i \) denotes the volumetric domain of the \( i^{th} \) element. To evaluate equation (24) the necessary quantities need to be sampled at a specific point, \( (\eta_1, \eta_2, \eta_3) \), in the interior of the element domain. This can be achieved by using the solution vector with equation (5) to obtain

\[
  E_{ij}^1 (\eta_1, \eta_2, \eta_3) = \frac{1}{2} \left( \frac{\partial N^P}{\partial x_j} \frac{\partial N^P}{\partial x_i} - \frac{\partial N^P}{\partial x_i} \frac{\partial N^P}{\partial x_j} \right)
\]

and

\[
  \Omega_{ij}^1 (\eta_1, \eta_2, \eta_3) = \frac{1}{2} \left( \frac{\partial N^P}{\partial x_j} \frac{\partial N^P}{\partial x_i} + \frac{\partial N^P}{\partial x_i} \frac{\partial N^P}{\partial x_j} \right)
\]
where $\Omega_{ij}$ are the biasing rotations. It should be noted that $E_{ij}$ and $\Omega_{ij}$ are sampled in the interior of the element domain where they are accurate. In general these quantities should not be considered accurate at nodal points or along element edges. Using equations (25) and (26), the deformation gradients at the element domain point $(\eta_1, \eta_2, \eta_3)$ are given as:

$$w_{ij}(\eta_1, \eta_2, \eta_3) = E_{ij}(\eta_1, \eta_2, \eta_3) + \Omega_{ij}(\eta_1, \eta_2, \eta_3)$$  \hspace{1cm} (27)

The biasing stresses, $T^L_{LM}$, at this point are then computed using equation (3) and all are combined via equation (23) to produce a values of the components of $\frac{\partial c_{LM}}{\partial \eta}$ at a point in the interior of the element under consideration.

A single element integral of equation (24) is computed by first subdividing the element into $m_1 \times m_2 \times m_3$ smaller sub-elements and sampling the $\frac{\partial c_{LM}}{\partial \eta}$ terms at the centroid of each of sub-domain. For a small enough domain, it may be assumed that the $\frac{\partial c_{LM}}{\partial \eta}$ terms are approximately constant, which leads to the approximation

$$\int_{\Omega} \frac{\partial c_{LM}}{\partial \eta} g_{1}^{\mu} g_{2}^{\nu} g_{3}^{\mu} d\Omega \approx \sum_{ij} \sum_{j} \sum_{k} \frac{\partial c_{LM}}{\partial \eta} \int_{\Omega} g_{1}^{\mu} g_{2}^{\nu} g_{3}^{\mu} d\Omega$$  \hspace{1cm} (28)

where $(\eta_1, \eta_2, \eta_3)$ denotes the centroid of the $(i, j, k)$ sub-element in the domain under consideration. The integral $\int_{\Omega} g_{1}^{\mu} g_{2}^{\nu} g_{3}^{\mu} d\Omega$ in equation (28) is evaluated exactly using the forms given by equations (16) and (18). The resulting formulas are very long and cumbersome and are therefore not listed here.

**Algorithm Verification**

The capabilities of the CAA tool been verified by performing acceleration sensitivity analyses on three reference problems and then comparing our calculated results with the experimental or theoretical results obtained in the references. The referenced examples could all be modeled as 2-dimensional problems. Two examples were plane stress problems, while the third example represented a plane strain problem.

The first reference problem analyzed was a classic force-frequency experiment carried out using a circular ST-cut substrate which was 31.75 mm in diameter. A 60 MHz SAW device was centered on the substrate which had an active area that was approximately 1.0 mm by 1.0 mm [4]. In this example a diametrical in-plane force was placed on the substrate and the change in resonant frequency of the SAW device was measured as a function of the azimuthal angle of the force with respect to the propagation direction of the SAW. Symmetry was used to reduce the size of the finite element mesh by a factor of two because only half of the disc needed to be modeled to accurately define the stresses generated near the active region of the device. In all cases, a convergence study was performed on the mesh to determine the optimal configuration for modeling the mechanical system. The finite element mesh at which convergence occurred was comprised of 432 quadratic serendipity quadrilaterals with a total of 1347 nodes. A representation of the mesh can be seen in Figure 4. Figure 5 shows a comparison of the results published by Sinha, et al., with those produced by the analysis tool. The percentage of error between the calculated and experimental results ranged from 9% to 23%. The primary source of error in modeling this example was the inability to accurately model a point force using the serendipity quadrilateral.

The second reference problem modeled the in-plane acceleration sensitivity of a SAW resonator on a rectangular substrate that was rigidly supported on all edges [5]. For this problem, the acceleration-induced frequency change had been theoretically predicted by Shick, et al. The variable in this experiment is the aspect ratio of the substrate. These devices operated at approximately 400 MHz and the active area was 1.0 mm. The initial substrate was a 19.05 mm square. Symmetry reduced the complexity of the finite element mesh by a factor of four, because only a quarter of the plate needed to be modeled to accurately portray the mechanical stress biasing the active area of the device. The finite element mesh of the quarter plate contained 300 quadratic serendipity quadrilaterals and contained 981 nodes. A model of the mesh for the entire plate can be seen in Figure 6. Beginning with a square substrate, aspect ratio (a/b) of 1:1, where 2a is the length of the substrate and 2b is the width, seven in-plane acceleration sensitivities were calculated with the aspect ratio of the substrate varying from 1:1 to 4:1. The results of this analysis are in Figure 7. Comparing the calculated results from the analysis tool with Shick's theoretical data at an aspect ratio of 1:1 the calculated data differed by 5%, while at 2:1 the calculated data differed by 17%. The difference in the 2:1 result occurred because Shick modeled a larger substrate in his
analysis (25.4 x 12.7, instead of 19.05 x 9.525).

The third example is a plane strain problem. In this experiment by Andres and Parker, it was shown that by properly massloading the backside of an all quartz package (AQP) SAW substrate that the bending stresses caused by a normal acceleration could be minimized [6]. Modeling this situation meant that the dimensions of concern were the length and thickness of the substrate which were 10.16 mm and 0.89 mm respectively, the length of the active SAW area was 0.5 mm. Since no dimensions were given for the masses, they were assumed to be 1.2 mm in length and three times as dense as quartz. The finite element mesh of the SAW substrate, masses, and glass frit can be seen in Figure 8. Symmetry reduced the complexity of the analyzed model by a factor of two. The mesh contained 270 quadratic serendipity quadrilaterals which had 929 nodes. The experiment was carried out as follows, two masses were attached to one of four symmetric positions on backside of the AQP SAW substrate and a normal acceleration was applied to the SAW device. The acceleration induced frequency shift was measured in the output of the oscillator under test and the normal vibration sensitivity was calculated. Once this process was completed, the masses were detached, repositioned in another of the sites and the process was repeated. Figure 9 shows a comparison between the experimental data and the calculated results. Although the quantitative results were not accurate because of insufficient data to model the physical problem, qualitatively the analysis of the problem yielded similar results with regard to the optimal placement of the weights to minimize acceleration sensitivity.

Conclusion

A quantitative analysis tool has been developed and demonstrated which calculates the acceleration sensitivity of a SAW traveling in an arbitrary piezoelectric substrate. This computer aided analysis tool performs four major functions to determine the acceleration sensitivity for any given problem. First, it generates a finite element mesh which accurately models the physical problem. Next, the static biasing problem is solved by calculating the nodal displacements caused by the forces applied to the mechanical system. The third function that the analysis tool performs is a calculation of the SAW mode shape based on Sinha and Tiersten's analytical technique. Finally, data from the previous steps are combine with the spatially varying effective elastic constants to calculate the acceleration of the SAW device.

One of the more interesting aspects of this analysis tool is that it allows the user to sample the stresses, strains, and rotations within any given element and then use that data in sophisticated integration schemes to improve model accuracy. The software has been proliferated on several different platforms including, a Cray supercomputer, a Sun workstation and a 486 laptop PC, demonstrating its flexibility.

The CAA tool achieved good agreement (5%-10%) with the experimental and theoretical examples where an accurate model of the physical example could be generated. All of the examples analyzed in this study were 2-D problems modeled on a 486 laptop PC. The CAA tool can also evaluate 3-dimensional problems, however, a workstation or larger CPU would be required.

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Figure 1. Amplitude envelope for first transverse mode in SAW transmission path and reflecting arrays

Figure 2. Amplitude envelope for second transverse mode in SAW transmission path and reflecting arrays

Figure 3. Amplitude envelope for third transverse mode in SAW transmission path and reflecting arrays
Finite Element Mesh of Resonator on Circular Disk:
# of Elements - 432
# of Nodes - 1347
Substrate Diameter - 31.75 mm
SAW Transducers:
F₀ - 60 MHz
λ - 52.63 um
# of electrodes/transduce
NA - 1.0 mm
L - 1.0 mm

Figure 4. Example problem for force-frequency experiment.

Finite Element Mesh of Resonator on Square Plate:
# of Elements - 300
# of Nodes - 981
SAW Transducers:
F₀ - 401.5 MHz
λ - 7.846 um
# of electrodes/transduce
NA - 1.0 mm
L - 1.0 mm

Figure 6. Example problem for in-plane acceleration using plane stress analysis.

Figure 5. Comparison of calculated and experimental results for force-frequency experiment.

Figure 7. Comparison of calculated and analytical results for in-plane acceleration plane stress problem.
Finite element mesh of SAW substrate, frit & masses:

- # of Elements - 270
- # of Nodes - 929

Substrate Length - 10.16 mm & Thickness - 0.89

SAW Transducers:

- $F_0$ - 900 MHz
- $\lambda$ - 3.51 µm
- Length - 0.5 mm

Figure 8. Example problem for the mass on substrate experiment using plane strain analysis.

![Insufficiently Stiffened Oscillator $\gamma_1$ at 150 Hz vs Weight Position](image)

Figure 9. Comparison of calculated and experimental results for the mass on substrate experiment [6].