Orders of Magnitude Reduction in Acoustic Resonator Simulation Times via the Wide-Band Rapid Analytical-FEA Technique

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***Abstract*— Spurious mode excitation is one of the largest obstacles towards the widespread adoption of piezoelectric MEMS resonator technology. This is in large part due to the lack of a wide-band and computationally efficient simulation solution to model the frequency response of complex 3D geometries. This paper presents the results from a solution to this problem: the Rapid Analytical/FEA Technique (RAFT). The RAFT combines the accuracy of FEA with the speed of analytical evaluation. For simulations with similar total degrees of freedom and frequency resolution, the RAFT simulation completes approximately 2,300 times faster than traditional FEA while accurately predicting the behavior of hundreds of spurious modes. The approach of the RAFT allows the use of FEA as an efficient design tool, rather than analysis tool, for in- and far-band spurious modes.**

Keywords— MEMS, Acoustic Resonator, Motional Resistance

I. INTRODUCTION (*Heading 1*)

Contour piezoelectric MEMS resonators are an attractive technology for next generation front-end radio frequency filters. They offer lithographically defined frequencies in an area-efficient footprint. However, contour piezoelectric MEMS resonators have not seen widespread adoption due in large part to spurious mode problems, which degrade resonator response.

Several efforts have been made to address spurious mode problems [1,2,3]. These modeling and design efforts have been restricted to frequencies near the intended mode, or restricted by material, mode type, or geometry. This is primarily due to simulation techniques and limited computational power. Full 3D multiphysics frequency domain sweeps in FEA packages can take a minimum of days to complete. Consequently, many designers resort to 2D simulations. These simulations often miss important out of plane behavior. Clearly, the community requires a 3D, rapid, broad frequency, computationally efficient solution for resonator simulation to enable design for spurious mode mitigation. Accordingly, this paper will present results from the Rapid Analytical/FEA Technique (RAFT). The RAFT simulation accurately predicts the scattering (S) parameters across a wide frequency span orders of magnitude faster than traditional FEA packages. These advantages will enable designers to predict the presence and severity of spurs in a time efficient manner. The devices in this paper are PZT-based, two-port, low frequency, contour mode resonators. However, the RAFT is capable of modeling a variety of resonant systems, such as gyroscopes, oscillators, ultrasonic motors, etc. The systems could be one-port, higher frequency, non-contour (e.g. thin-film bulk acoustic resonators (FBAR)) or non-PZT based.

II. METHOD

The well-known modified Butterworth van-Dyke (mBVD) model is the foundation of this technique. Each "motional" path, consisting of a motional inductance, resistance (R_m), and capacitance, represents the behavior of a single mode. These elements are electrical representations of the lumped resonator mass, spring, and damper. To arrive at the lumped mass and spring, the kinetic and elastic energies of the lumped and continuous resonator systems are compared. The damping is found by assuming or measuring mechanical quality factor (Q_m). Placing motional arms in parallel, as in Fig. 1, superimposes the modes to obtain the frequency response of the resonator.

While the mBVD model is not new, its wide-band design capabilities have not been fully utilized. Until now, a general expression for the modal force, and subsequently the R_m, of the resonator, of an arbitrary mode of an arbitrary resonator did not exist. This is the enabling breakthrough of this simulation technique, and is achieved by comparing elastic energies in the real and lumped systems. By comparing energies, the need for a specific expression for force or strain is eliminated. The closed form expression for R_m separates the simulation of the

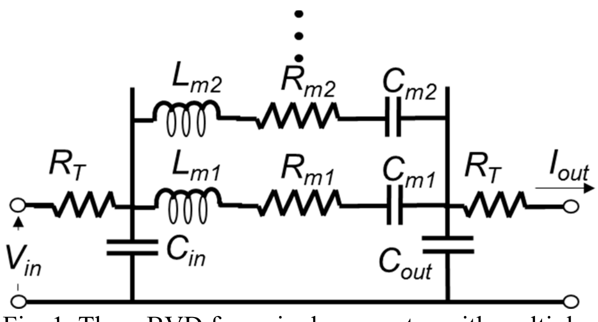

Fig. 1. The mBVD for a single resonator with multiple mechanical modes.

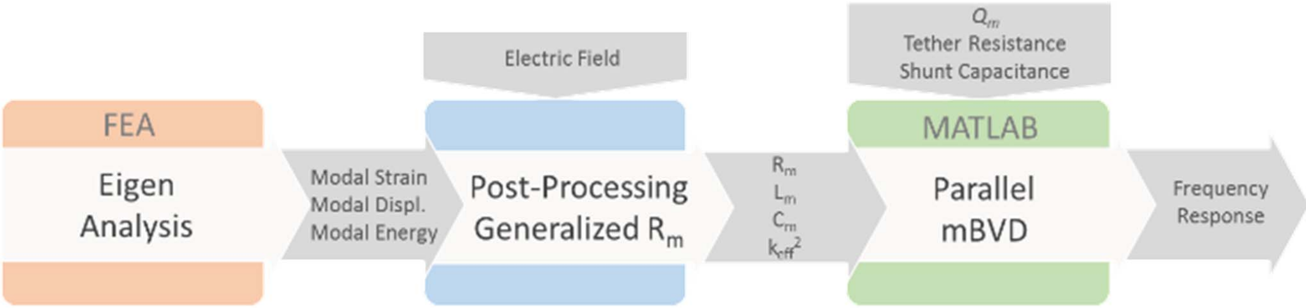

Fig. 2. Overview diagram for the RAFT

mechanical and piezoelectric domains for low-moderate coupling resonators. The complex mode shape, modal energy, and strain may be obtained from relatively fast Eigen frequency simulations. This information is then processed by an analytical software package. After assigning Q_m, the motional parameters of each mode are returned. The full S parameters are then calculated based on R_m, Q_m, and material properties. An overview of this process is presented in Fig. 2.

The closed form expression for R_m is given by

$$R_m = \frac{k_m}{Q_m \omega_n \left| \int_{V_{in}} \boldsymbol{e}^t \cdot \boldsymbol{\nabla}\overline{\phi} \cdot \boldsymbol{S}_n dV \int_{V_{out}} \boldsymbol{e}^t \cdot \boldsymbol{\nabla}\overline{\phi} \cdot \boldsymbol{S}_n \, dV \right|} \quad (1)$$

Where k_m is the modal spring, ω_n is the natural frequency, V_{in} refers to the volume of the piezoelectric material affected by the input port's electric field, e is the piezoelectric coefficient matrix, S_n is the six dimensionalcompressed strain vector in Voigt's notation derived from a unity normalized mode shape, $\overline{\phi}$ is the unity normalized vector field, and A_{out} is the area of the electrode on the output port. For the devices in this paper, the electrodes may be approximated as perfect parallel plate capacitors with electric field in the 3 direction. Additionally, the electrodes are symmetric along the device midplane defined by a vector orthogonal to the tethers and surface of the wafer. Using these assumptions, (1) reduces to

$$R_m = \frac{k_m}{Q_m \omega_n \left(\int_{A_{el}} \boldsymbol{e}_{3i} \cdot \overline{\boldsymbol{S}}_n d\boldsymbol{A} \right)^2} \quad (2)$$

Where $\overline{S}_n$ is the strain in the piezoelectric layer average through the thickness. This is the expression used in the RAFT for resonators with parallel plate electrodes. A mechanical Eigen analysis will return the total energy of the system. After equating the potential energies of the lumped and continuous resonators, a value for k_m is reached. A modal displacement must be chosen to define the modal spring relative to, and is chosen to be the point of largest displacement for each mode. ω_n and the strain may be taken directly from and FEA, and the e matrix is a material property. Finally, a value for the Q_m must be assumed or chosen. Values for L_m and C_m may then be calculated by the definition of Q_m using electrical equivalent parameters, which for parallel plate electrodes are

$$L_m = \frac{m_m}{\left(\int_{A_{el}} \boldsymbol{e}_{3i} \cdot \overline{\boldsymbol{S}}_n d\boldsymbol{A} \right)^2} \quad (3)$$

$$C_m = \frac{\left(\int_{A_{el}} \boldsymbol{e}_{3i} \cdot \overline{\boldsymbol{S}}_n d\boldsymbol{A} \right)^2}{k_m} \quad (4)$$

Where m_m is the modal mass. The parameters for the motional path are now known. The tether resistances and shunt capacitances then must have their values set, and the system may be simulated.

The effective electromechanical coupling factor may be calculated now. Using (1), the most general form is

$$k_{eff}^2 = \frac{1}{\frac{C_0}{C_m} + 1} = \frac{1}{\frac{k_m C_0}{\left| \int_{V_{in}} \boldsymbol{e}^t \cdot \boldsymbol{\nabla}\overline{\phi} \cdot \boldsymbol{S}_n dV \int_{V_{out}} \boldsymbol{e}^t \cdot \boldsymbol{\nabla}\overline{\phi} \cdot \boldsymbol{S}_n \, dV \right|} + 1} \quad (5)$$

Using the parallel plate assumption turns (5) into

$$k_{eff}^2 = \frac{1}{\frac{k_m C_0}{\left| \int_{A_{in}} \boldsymbol{e} \cdot \overline{\boldsymbol{S}}_n \, dA \int_{A_{out}} e \cdot \overline{\boldsymbol{S}}_n dA \right|} + 1} \quad (6)$$

For one port resonators, C_o is the shunt capacitance. For two port resonators, C_o is found by placing the two shunt capacitors in parallel to create an effective one port resonator.

III. Results

The model was validated against resonators fabricated in PZT-on-Silicon process [4]. The material stack consists of 1 µm buried silicon dioxide, 10 µm of silicon, 300 nm of silicon dioxide, 125 nm of platinum, 0.5 µm of PZT, and 50 nm of platinum. A ZVB-8 network analyzer terminated to 50Ω and calibrated using a through, short, open, and load standard (GGB CS-5) was used to measure the resonator's S parameters. One resonator was designed to optimally excite the (1,1) mode of

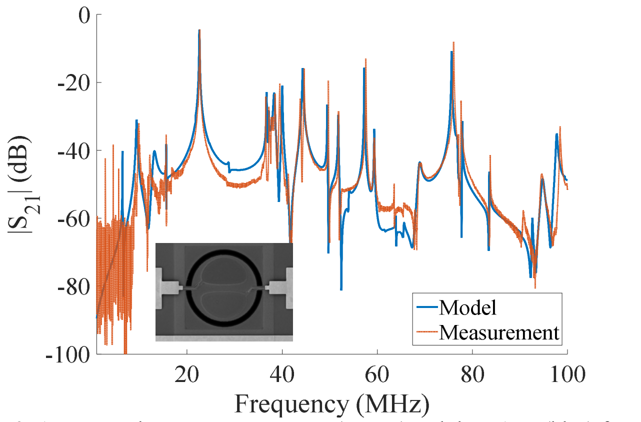

Fig. 3. Agreement between measurement (orange) and the RAFT (blue) for a disk resonator (inset). There were 103 modes in this bandwidth. The plotted resonator data was mathematically terminated to 300 Ω.

transverse disk flexure [5,6] (Fig. 2), which has shown an insertion loss of -1 dB in recent a recent publication[7,8]. The other was designed for beam length extension (Fig. 2), a commonly utilized mode.

Measured properties and designed geometries were used in the model simulations. Elastic moduli of the materials in the PZT-Silicon stack were independently measured [9]. The e_{31} values in the model fell within a range extracted from cross-wafer cantilever test structures. Densities were taken to be bulk values. Geometric dimensions from CAD were decreased for frequency agreement, resulting in a 0.5 µm decrease in disk radius and beam width, which is within fabrication tolerance. mBVD values for the shunt capacitor and tether resistances were extracted from S parameter measurements by analyzing the frequency response away from resonance.

The disk flexure device was measured from 1 to 100 MHz, with the designed mode at 20.65 MHz. The comparison between the measured and predicted S parameters may be seen in Fig. 3. The RAFT model was able to accurately predict the device behavior across the bandwidth. The spurious modes in this simulation had measured and fitted Q_m ranging from 50 to 1700. Some modes had fitted Q_m due to measurement difficulty from loss or frequency spacing. Across the lowest loss modes, the error in predicted S_{21} at resonance was 1.5 dB.

The measurement on the beam extension device was taken from 1-80 MHz, with the designed mode at 20.7 MHz. Agreement between measurements and the results from the analytical-FEA technique is presented in Fig. 2. Fitted and measured Q_m for the beam ranged from 50 to 1500, and average error between measure and model across the lowest loss peaks was 1.8 dB.

The time from simulation start to generation of S parameters for the disk was 11.7 minutes. The total number of degrees of freedom was ~460,000. In this frequency span there were 103 modes. The beam had a total of 345,000 degrees of freedom, which took 9.9 minutes to simulate. There were 247 modes in the frequency range simulated.

To illustrate the speed of this method, a full multiphysics simulation was run in COMSOL. While simulating the same

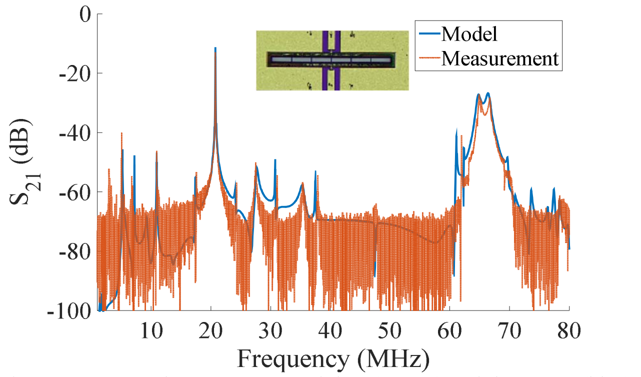

Fig. 4. Agreement between measured data (orange) and the RAFT (blue) for a beam extension resonator (inset). There were a total of 257 modes in this frequency span.

frequency span would take a prohibitively long time, several shorter runs were performed, and the results were linearly extrapolated for comparison. Table 1 compares the time (t_{COMSOL} and t_{RAFT}) to simulate a 99 MHz frequency span with various point densities for models with 460,000 degrees of freedom. For context, a frequency resolution of 1 kHz would place approximately 35 points in the bandwidth of the intended mode of Fig. 1 at 20 MHz.

TABLE I. SIMULATION TIMES FOR 99 MHZ BANDWIDTH

Points	*(Frequency Points/MHz)*	*Frequency Resolution*	*COMSOL Simulation Time*	*RAFT Simulation Time*	t_{COMSOL}/t_{RAFT}
9900	100	10 kHz	~10d 5h 30m	11.7m	1259
49500	500	2 kHz	~54d 10 h	11.7m	6697
99000	1000	1 kHz	~112d 7h	311.7m	13820

IV. DISCUSSION

There are several advantages to this approach to simulation in the context of spurs. First, all simulations may be performed in full 3D with high mesh densities, capturing out of plane behavior and complex behavior such as tether response. Secondly, it may be used as a design tool to parametrically explore how design parameters affect spurs far away from the intended mode. Third, commercially available methods scale linearly with the number of frequency points, since full equations of state must be solved at every point. The RAFT simulation method scales with the number of modes, which is advantageous in contour resonators where there are many modes which are electrically detectable. Additionally, modal information is directly available to analyze the contribution of particular modes to the response. This allows designers to debug spurious modes and intelligently design around them.

The simulations in this paper were low frequency and utilized capacitors that could be approximated as parallel plate. In higher frequency topologies, such as devices with interdigitated electrodes, it may be desirable to simulate t he electrical field in a separately, which would slightly increase the simulation time. However, the R_m equation presented in this paper and the resulting methodology have been generalized for arbitrary modes in arbitrary geometries and materials, and can provide significant decrease in simulation times. This will decrease reliance on expensive parametric fabrication, make FEA a viable tool for pre-fabrication analysis, enable wide band spurious mode design, allow designers to explore novel high-coupling modes.

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