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Finite Element Analysis of BAW resonators: a matter of model dimensionality?

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***Abstract*— We investigate the numerical predictions of the Finite Element Method for bulk acoustic wave resonators. A conventional 2D model is used to calculate major performance indicators of the piezoelectric resonators, such as energy confinement (Q-value) and effective piezoelectric coupling K_{eff}. The results are compared to experimentally evaluated values. We show that these indicators can be accurately predicted by using a 2D model in combination with appropriate boundary conditions.**

Keywords—bulk acoustic wave resonators, Finite Element Method

I. Introduction

Modern filter devices increasingly rely on high-performance bulk acoustic wave (BAW) resonators as their fundamental building blocks. Major performance indicators of the piezoelectric resonators include energy confinement (Q-value), effective piezoelectric coupling (K_{eff}) or spurious mode content [1]. Although a limited analytical analysis of the device is possible [2], an accurate analysis of scattering phenomenon and the evaluation of the above-mentioned indicators requires numerical tools based on the Finite Element Method (FEM). As the resonators are 3D structures, which can exhibit irregular (nonsymmetric) shapes, 3D FEM models are in general more accurate but numerically costly and hence often impracticable [3]. In this work we investigate the possibilities and prospects of 2D approaches, which are more efficient and practicable.

II. Model Setup

A typical schematic cross-section of a BAW resonator is shown in Fig.1. The active area consists of a piezoelectric layer sandwiched by a top electrode and a bottom electrode. For solidly mounted resonators (SMR) an acoustic mirror is used to create the desired standing wave in the piezoelectric layer and prevent the energy leakage into the substrate material.

A. Governing equations

Two physical domains are coupled in a piezoelectric device: the acoustic and the electrical domains [3]. The governing

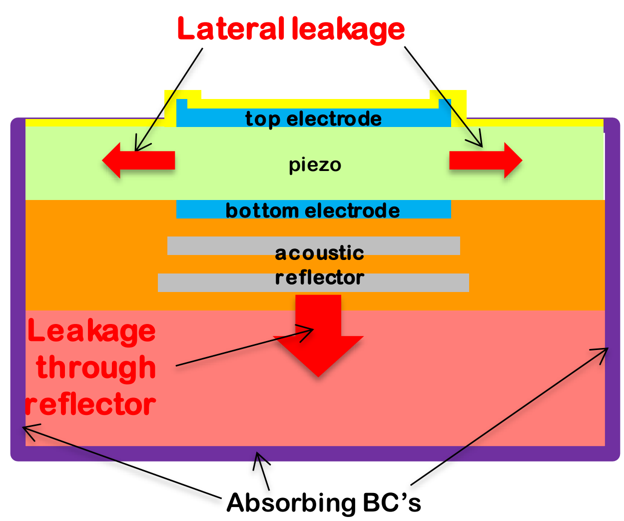

Fig. 1: Typical cross-section of a Solidly Mounted Resonator consisting of a piezoelectric layer, top and bottom electrodes, and an acoustic mirror. Energy leakage and boundary conditions (BC's): the absorbing BC's should prevent the reflections of acoustic waves at the truncations of the system.

equations for the acoustic / mechanical domain are given by the equation of motion:

$$\nabla \cdot \mathbf{T} = \rho \frac{\partial^2 \mathbf{u}}{\partial t^2},$$

where $\mathbf{T}$ denotes the mechanical stresses, ρ the density and $\mathbf{u}$ the mechanical displacements. In the electrical domain the electrostatic approximation can be used, and the governing equations are given as [3]:

$$\nabla \mathbf{D} = 0,$$

where $\mathbf{D}$ denotes the dielectric displacement. The two domains are coupled by the constitutive equations:

$$\mathbf{T} = c_E\mathbf{S} - \mathbf{eE},$$

$$\mathbf{D} = \varepsilon_S\mathbf{E} + \mathbf{eS},$$

where **S** and **E** denote mechanical strain and electric fields, respectively, c_E , and **e** are the mechanical stiffness and piezoelectric tensor, and ε_S is the dielectric constant at constant strain. These equations are normally implemented in standard FEM solvers, such as Comsol, Ansys etc. and can be solved using proper boundary conditions.

B. Boundary conditions for SMR

As depicted in Fig.1, the active area of a SMR is embedded in a larger solid body, and the resonating piezoelectric layer interacts with this volume. Since the stresses and displacements must remain continuous at the end of the active area, this interaction leads to energy leakage, or to the generation of propagating modes [4]. In the real structure, these propagating modes largely get absorbed by the surrounding medium or get scattered into every possible direction and, hence, don't interact with the resonator constructively. For a numerical solution by FEM, this domain thus needs to be truncated and reflection from the boundaries must be avoided by choosing appropriate absorbing boundary conditions (BC's), as shown in Fig.1.

Besides the acoustic, also the electrical BC's need to be defined. In the FEM simulations usually the frequency response of the device is calculated to an electrical stimulus. The simplest approach is to set the interfaces of the electrodes and piezoelectric layer to be equipotential surfaces, bound to an external terminal with constant power or Voltage.

III. Numerical solution with FEM in 2D

A. Simulations in 2D and comparison with experimental data

The ultimate aim in pursuit of simulations is an appropriate description of the physical reality using numerical models. This in return will lead to a better understanding of the underlying physics as well as to a prediction of the behavior of new structures / geometries. Using comprehensive full 3D simulations, experimental reality can be matched, described or predicted. Full 3D simulations of BAW devices are fundamentally possible with clusters, or comparable high-performance computers, but the corresponding memory requirement of these simulations are still demanding and beyond of the practicality of everyday simulations [3].

In this work, we investigate the possibilities and prospects of 2D approaches, which are more efficient and practicable, to calculate the major performance indicators of the piezoelectric resonators. Let us first consider the evaluation of Q-values. According to Ref [4] the quality factor is a measure of the loss in the system and can be expressed as the ratio of the total energy (E_{tot}) to the energy loss (ΔE) in a full cycle:

$$\mathrm{Q} = 2\pi\frac{E_{tot}}{\Delta E},$$

and the total loss of the resonator can be summed up from multiple loss mechanisms:

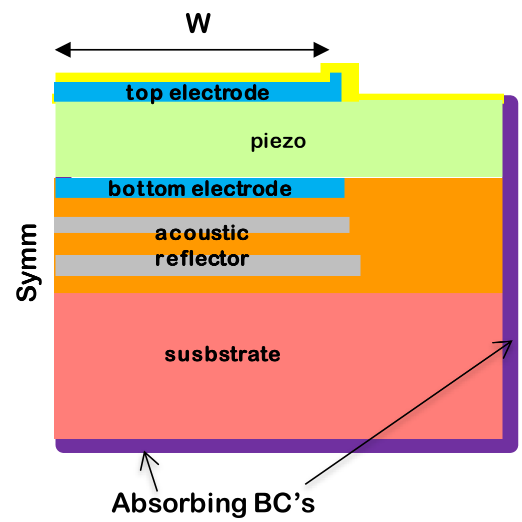

Fig. 2: Energy leakage and boundary conditions (BC's) for a SMR with raised frame or border ring. The absorbing BC's should prevent the reflections of acoustic waves at the truncations of the system.

$$\frac{1}{Q_{tot}} = \frac{1}{Q_{vert}} + \frac{1}{Q_{leak}} + \frac{1}{Q_{mat}} = \frac{1}{2\pi}\left[\frac{\Delta E_{vert}}{E_{tot}} + \frac{\Delta E_{leak}}{E_{tot}} + \frac{\Delta E_{mat}}{E_{tot}}\right],$$

where Q_{vert}, and Q_{leak} are the vertical and leaked energy losses according to Fig. 1 and Q_{mat} denotes the material dissipation. The great advantage of this formalism is that the calculation of these quantities does not require the use of a 3D model. According to Fig. 1, the energy losses ΔE_{vert}, and ΔE_{mat} are proportional to the area of the resonator, whereas ΔE_{leak} is obviously proportional to the circumference. Using a simple 2D model, as depicted on Fig.2, they can be calculated for unit area and for unit length and adjusted in post-processing for the correct area and circumference.

Although, the effective coupling coefficient K_{eff} can also be calculated from energy considerations [4], we would like to demonstrate that it is possible to use a 2D model to accurately describe the experimentally observed behavior. The effective coupling coefficient K_{eff} can be evaluated from the admittance, for example, by using the series and parallel resonance frequencies f_s, f_p [4]:

$$K_{eff}^2 = \frac{\pi}{2}\frac{f_s}{f_p} cot\left(\frac{\pi}{2}\frac{f_s}{f_p}\right),$$

In experiments, the variation of the width of the border ring (Fig.2) can be used to optimize the resonator performance (Q-values, for example), which results in the variation of the effective coupling coefficient as well. The correct ratio of the series and parallel resonance frequencies f_s , f_p can be approximated with a 2D FEM model, if the ratio of the active area and the area of the border ring is the same as for the experiment. In particular, this can be achieved by choosing the width of the model W as one quarter of the effective real resonator width and using the correct width for border ring, as depicted in Fig. 2.

Predictions were made for a resonator with 150x150 μm^2

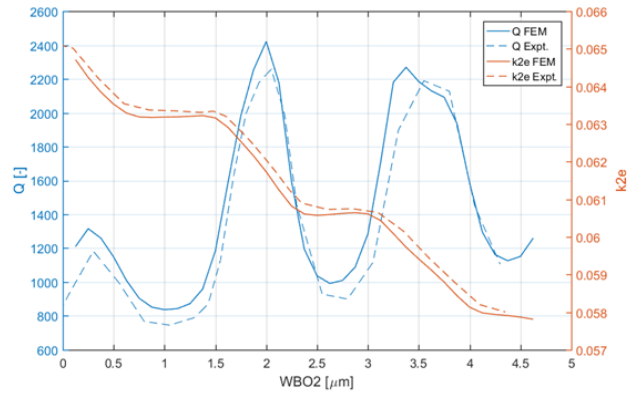

Fig. 3: Quality factor, Q, and effective coupling, k2e, calculated with the 2D FEM model as a function of the width of the raised frame, WBO2, and compared to experimental data from a regular 3D device.

area and compared to experimental data. Material properties, such as elasticity tensors and attenuation were evaluated beforehand and tested on numerous test cases. In experiments, the width of the border ring (Fig.2) was varied to optimize the resonator performance. As the comparison in Fig.3 shows, the Q-values from the energy calculation using the 2D FEM follow the experimental data remarkably well. The effective coupling coefficients were evaluated from the admittance of the 2D FEM simulation and follow the experimental results equally well.

IV. Conclusion

In conclusion, we have numerically predicted performance indicators of BAW resonators (Q, K_{eff}) using a 2D FEM model and compared the results to experimental data from regular 3D devices. The comparison showed, that by using properly chosen geometry and boundary conditions, these values can be predicted with high accuracy using the 2D FEM approach. Our work demonstrates that by using a 2D FEM model, most important performance indicators can be accurately predicted at much lower expenses than using 3D FEM approaches.

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