# Optimization of BAW resonator performance using combined simulation techniques

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## Abstract

Filters based upon bulk–acoustic–wave (BAW) resonators are attractive for a variety of RF applications. To master the ambitious specifications and to facilitate a fast and cost economic design, we present an efficient simulation strategy combining different modeling approaches. As the first step, a 1D transmission line model (Mason model) is used for constructing the layer stack to meet the desired resonance frequencies and bandwith. Second, the system of Newton's equation of motion and Maxwell's equations coupled by the piezoelectric effect is solved by FEM simulations. Thus, the lateral structure, e. g. specific border regions, can be designed to maximize the Q factor and to minimize the excitation of spurious modes. The theoretical predictions are excellently confirmed by experimental results.

## 1 Introduction

Bulk acoustic wave (BAW) resonators are of increasing interest for a variety of RF system applications. Compared to SAW and ceramic filters, they offer superior performance and significant advantages in chip size and processing costs, respectively [1]. To master the challenging specifications, e. g. the purity of the resonance and a large Q factor, highly accurate numerical simulations are an indispensable tool to analyze the device behavior and to optimize its performance. For that purpose, we present an efficient simulation methodology for designing and optimizing BAW resonators.

## 2 BAW resonators

Infineon's solidly mounted BAW resonators (fig. 1) comprise a piezoelectric layer above an alternating series of oxide and tungsten layers acting as an acoustic mirror. At the mechanical resonance frequency $f_s$, the impedance (fig. 2) of the device is at its minimum (series resonance condition). A maximum impedance is observed at the so–called parallel resonance frequency $f_p$ where the dielectric and the mechanically induced displacement currents nearly balance. As the continuity conditions at the resonator edges cannot be satisfied by a constant displacement amplitude in the resonator (piston mode), an additional border region with an overlap oxide is introduced [2]. It enables a continuous combination of the displacement distributions, thus facilitating the piston mode and reducing the content of spurious modes (cf. fig. 1).

The decisive requirements for BAW resonators to be used in RF filters are a precise control of the resonance frequencies, a large Q-value, a good piezoelectric coupling, and the purity of the resonance, i. e. the lack of spurious modes. Therefore, the structures need to be optimized with respect to an optimum confinement of the mechanical energy in the piezoelectric layer.

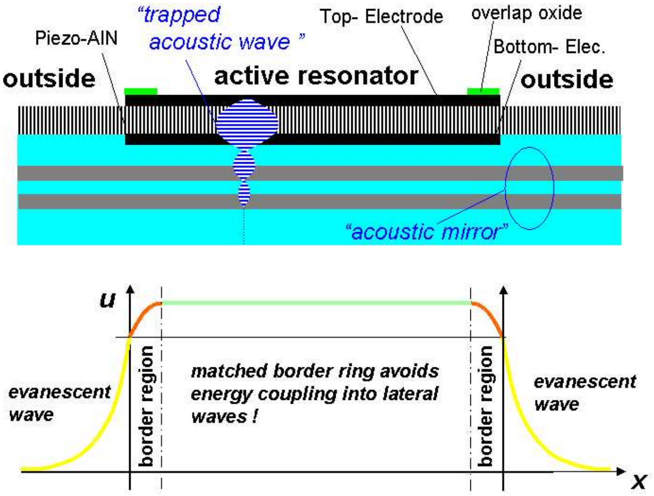

Figure 1: BAW resonator structure (above). The schematic in the lower part illustrates the principle of a border region with an overlap oxide which is introduced to suppress spurious modes.

## 3 Simulation Strategy

For practical device development, the first step consists in simulations based upon the Mason model to construct a suitable layer stack with the desired resonance frequency, effective coupling constant $k_{\mathit{eff}}^2 = \pi^2/4 \cdot (f_p^2 - f_s^2)/f_p^2$ and mirror reflectivity. The lateral design, in particular the border region width and the mirror termination, is analyzed by 2D FEM simulations to optimize the Q value, the effective coupling and the content of spurious modes.

### 3.1 Mason Model

The Mason model is a 1D transmission line model [3], where the mechanical displacement $\boldsymbol{u}$ is assumed a superposition of upward and downward travelling waves in each layer $j$

$$\boldsymbol{u}_j = \boldsymbol{u}_{j+}e^{ik_jz} + \boldsymbol{u}_{j-}e^{-ik_jz} \tag{1}$$

with $k_j$ representing the wave vector in the respective material. The expansion coefficients $\boldsymbol{u}_{j\pm}$ are determined by the continuity conditions at the interfaces and the vertical boundary conditions.

### 3.2 FEM Simulations

FEM simulations of BAW devices are based upon solving Maxwell's equations of electrostatics

$$\mathrm{rot}\boldsymbol{E} = 0 \quad \text{and} \quad \mathrm{div}\boldsymbol{D} = 0 \tag{2}$$

and Newton's equation of motion in the frequency domain

$$-\omega^2\rho\,\boldsymbol{u} - i\omega\gamma\,\boldsymbol{u} = \nabla\mathcal{T} \;=\; \sum_{i,j} \boldsymbol{e}_i \,\frac{\partial \mathcal{T}_{ij}}{\partial x_j} \tag{3}$$

where the force density effecting the mechanical displacement $\boldsymbol{u}$ is given by the divergence of the stress tensor $\mathcal{T}$. The constitutive relations for the stress and the dielectric displacement $\boldsymbol{D}$ are

$$\mathcal{T} = c\mathcal{S} - e^T\boldsymbol{E} \quad \text{and} \quad \boldsymbol{D} = e\mathcal{S} + \varepsilon\boldsymbol{E} \tag{4}$$

The electro–acoustic coupling is represented by the $3 \times 6$ piezoelectric tensor $e$ which — dependening on crystal symmetry — has 1 to 4 independent coefficients. In addition to a careful calibration of the material parameters, a suitable choice of the boundary conditions to suppress artificial reflections at the egdes of the simulation domain is an indispensable prerequisite. The results presented here are calculated using the simulator CAPA [4].

## 4 Application Example

Employing the 1D Mason model, the layer stack is designed such that the piezolayer thickness and the mirror reflectivity (fig. 2, inset) suits to the desired resonance frequency and bandwidth (fig. 2). FEM simulations reveal the displacement distribution of the main mode (fig. 5, left) and the behavior of a lot of additional modes (fig. 3), e. g. the so–called overlap modes (resonance of the border region, cf. fig. 5, right). Simulating the impedance characteristics for various resonator designs (fig. 2), the border region can be optimized with respect to a maximum Q-factor and a minimum content of spurious modes (fig. 4). The simulation results are excellently confirmed by the experiments.

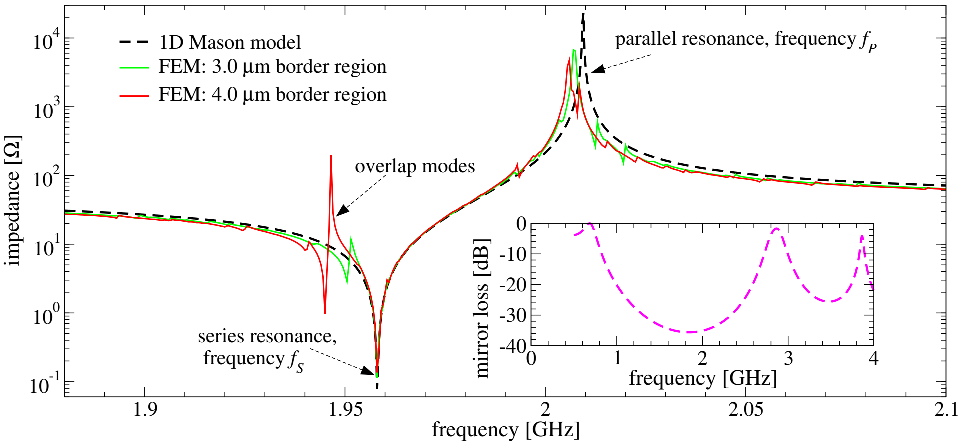

Figure 2: 1D Mason model and FEM simulations of the impedance of a BAW resonator for different widths of the border region. The inset shows the transmission losses of the acoustic mirror (Mason model). Low values indicate high mirror reflectivity.

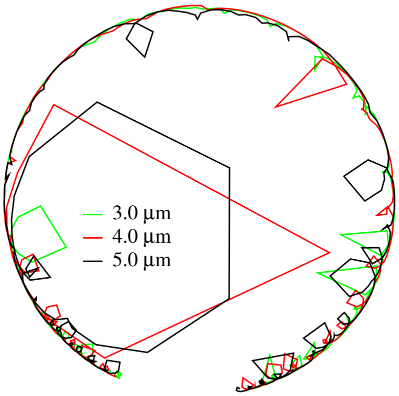

Figure 3: Smith chart of the impedance plotted in fig. 2. Each of the inner circles (partially represented by polygons due to the discrete set of frequency points) corresponds to an additional mode.

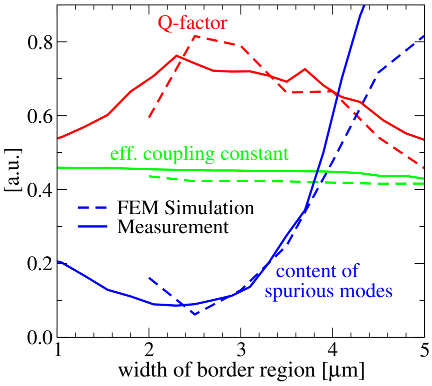

Figure 4: Typical device characteristics for different lateral designs (width of border region). Solid lines refer to measurements, dashed lines represent FEM simulation results.

## 5 Conclusion

An efficient simulation strategy for designing BAW resonators has been presented. It is based upon a 1D transmission line model and coupled electro–acoustic FEM simulations and has proven to be a valuable method for design optimization, as it accurately predicts the decisive characteristics of the devices.

## References

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[4] R. Lerch, H. Landes, M. Kaltenbacher, CAPA User Manual, Release 3.4, University of Erlangen, Germany, 2000

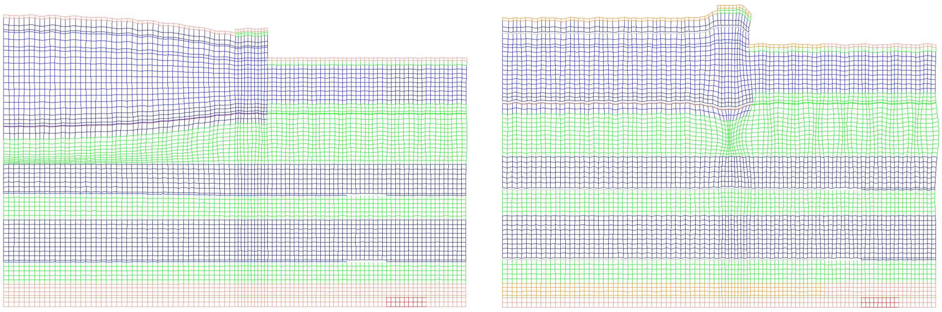

Figure 5: Displacement distribution at the series resonance frequency (left) and displacement distribution of the overlap mode (right). Exploiting symmetry, only the right hand half of the structure is shown.