Bulk acoustic wave resonators 3D simulation

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***Abstract*— This article discusses numerical simulations of thin film bulk acoustic wave resonators. FBAR simulation with 1D analytical model permits to quickly determine resonator layers thicknesses that correspond to the objective resonant frequency. 3D finite elements method permits to investigate the effect of the electrode shape on the spurious modes that are present in the electrical impedance. In order to reduce or to suppress those modes, solutions have to be investigated.**

I. INTRODUCTION

Acoustic waves in elastic solids are utilized in numerous applications in signal processing, including frequency generation, control and filtering in modern wireless communication systems. Resonators and band pass filters based on bulk acoustic waves (BAW) are extensively used in wireless applications such as cellular phones as they often feature superior performance in comparison to competing technologies (ceramic and surface acoustic wave devices). The physical phenomenon underlying the operation of BAW devices is the piezoelectric effect. In piezoelectric materials the electric and mechanical fields are coupled, enabling the excitation of acoustic waves by electric field. Since the velocity of acoustic waves in elastic solids is generally five orders of magnitude lower than that of the electromagnetic waves, the dimensions of the acoustic wave devices are in the same proportion smaller than devices directly employing the electromagnetic waves, e.g., ceramic filters.

II. PIEZOELECTRIC EFFECT

Piezoelectricity is the ability of certain crystals to generate a voltage in response to applied mechanical stress (direct effect) or to mechanically deform with applied electric field (converse effect). It is a coupling between electrical and mechanical problems. It can be modeled into coupled equations (1).

$$\begin{aligned} T_{ij} &= c_{ijkl} \cdot S_{kl} - e_{ijk} \cdot E_k \\ D_k &= \varepsilon_{kl} \cdot E_l + e_{ijk} \cdot S_{ij} \end{aligned} \qquad (1)$$

With :

T : mechanical stress (Pa) E : electric field (V/m)

S : mechanical strain D : electric displacement(C/m^2)

c : compliance tensor (Pa) ε : permittivity tensor (F/m)

e : piezoelectric tensor (C/m^2)

Solving piezoelectric Christoffel equation demonstrates that, with a longitudinally applied electric field, three plane waves with orthogonal polarizations can propagate in the same direction with different velocities [1]. So-called quasi-longitudinal wave propagates in the electric field direction and shear waves propagate in the orthogonal plane.

Hexagonal crystals, like AlN or ZnO, have a six fold rotation symmetry. It leads to such a compliance tensor that quasi shear waves are very weakly coupled. This approximation is considered in equivalent circuit models (e.g. Mason or Butterworth-Van Dyke). It is also considered in our 1D analytical model.

III. 1D ANALYTICAL MODEL

A. Simulation method

If only the active resonator area (Fig. 1) under top electrode and longitudinal thickness extension mode are considered, equations (1) can reduce into (2). The coupled system can then be solved analytically.

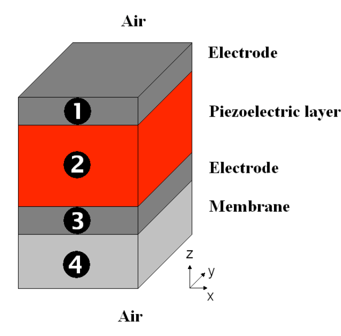

Figure 1. Active area of a suspended resonator

For longitudinal propagation (z-direction) piezoelectric equations are :

$$T_{33}(z) = c_{33}^{E} \frac{\partial u_z}{\partial z} - e_{33} E_z(z)$$
$$D_z(z) = \varepsilon_{33}^{S} E_z(z) + e_{33} \frac{\partial u_z}{\partial z} \qquad (2)$$

With plane waves, mechanical displacement u_z is formulate for each layer i (i = 1 to 4) as :

$$u_{z,i} = a_i e^{-jk_i z} + b_i e^{jk_i z} \qquad (3)$$

Where a_i and b_i are constants to be determined, and k_i propagation constant for layer i in z-direction. On layer boundaries, u_z and T_{33} are continuous. It permits to determine a_i and b_i and to plot the mechanical displacement. In time harmonic formulation, $I = j\omega Q$. On the piezoelectric material/metal interface, D_z is continuous, then $Q = S.D_z$ (with S = electrodes surface). The voltage U in piezoelectric layer is determined by E_z integration along considered layer thickness. The resonator impedance Z is :

$$Z = \frac{U}{j.\omega.S.D_z} \qquad (4)$$

E_z and D_z are coupled with equation (2). Then U is D_z function and leads to Z simplifications.

B. *Mechanical displacement modes display*

Our 1D analytical simulation tool permits to plot mechanical displacement. This is a very convenient way to understand physical phenomenon underlying longitudinal modes dispersion.

On Fig. 2, the first and the second modes of a suspended resonator are plotted.

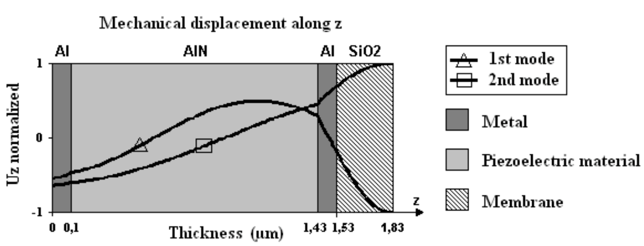

Figure 2. First and second mechanical displacement modes of a suspended resonator

We can notice that the first resonance is a λ/2 mode and the second is nearly a λ mode. The acoustic wave get in the membrane and the mechanical vibration mode takes place in the whole structure. It demonstrates the effect of the membrane on the resonant frequency. Generally, membrane tends to be thin in order to reduce mechanical losses.

The example on Fig. 3a and 3c shows how acoustic isolation between resonator and substrate is improved with the number of Bragg layers and how the acoustic wave is attenuated.

On Fig. 3b, mode plotting permits to understand how cavity modes can appear at low and high frequencies in solidly mounted resonator (SMR).

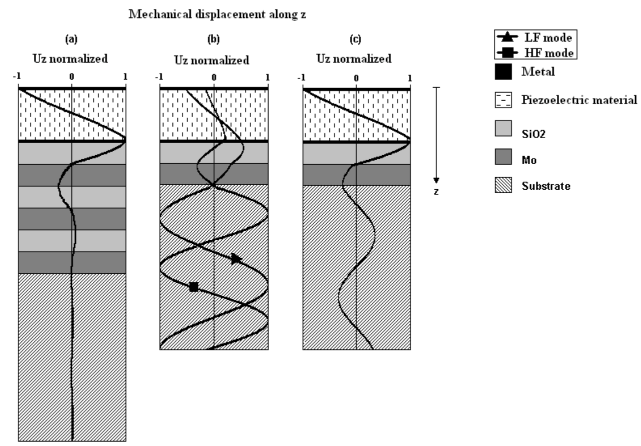

Figure 3. Mechanical displacement modes of a SMR structure

On Fig. 4, the first, second and third vibration modes for stacked crystal filter (SCF) are plotted. The first resonance is a λ/2 mode. Each resonator works at a quarter of the wavelength. The second resonance is a λ mode and each resonator works at λ/2. This is the maximum coupling frequency where losses are minimum. There is no coupling with the third mode because electrical potential and mechanical displacement are out of phase. The 2λ mode does not exist because the three electrodes can not be at the same potential.

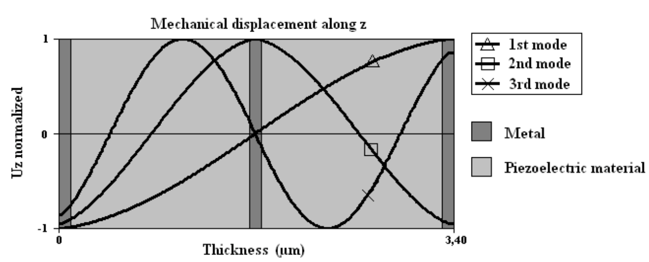

Figure 4. Mechanical displacement modes of a CRF structure

This 1D analytical simulation tool is very convenient to understand physics phenomenon underlying mechanical displacement modes dispersion in bulk acoustic wave resonator. It permits to quickly determine layers thicknesses that correspond to the objective resonant frequency. However, it does not permit to predict spurious modes that may appear with lateral direction mode coupling. It does not take into account the excitation and resonator coupling or electrical or mechanical coupling between resonators. The 1D approximation becomes too restrictive then we need a 3D simulation tool.

IV. 3D NUMERICAL FEM MODEL

3D calculation cannot be performed with simplified equations. The coupled field equations system (1) has to be solved with a powerful numerical simulation tool. We are using 3D simulation software based on the finite element method (FEM). In FEM, the complete problem domain is discretized. It permits to formulate the physical domain into finite dimensions. From an infinite point set, we obtain a finite element set compounds of nodes and lines. To keep the problem size finite, the physical domain needs to be truncated. This truncation introduces artificial boundaries where artificial boundary conditions are considered. This may induced modeling errors.

We have implemented the piezoelectric problem resolution in the existing 3D FEM electromagnetic software EMXD developed at Xlim for several years. But, to validate our first results, we performed some simulations with the commercial software ANSYS Multiphysics.

A. ANSYS Multiphysics-EMXD comparison

We performed the analysis of the suspended resonator presented in Fig. 5 with both ANSYS and EMXD, and with the same mesh.

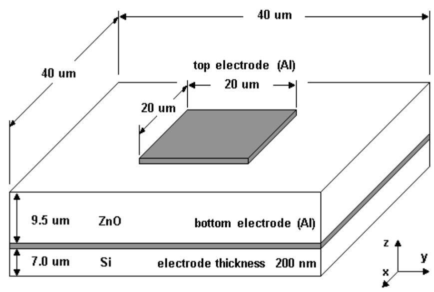

Figure 5. Suspended resonator for results comparison

We found that there is a good agreement between those two softwares (Fig. 6), but EMXD results are obtained with a reduced calculation time thanks to frequency parametrisation and highly parallel computing.

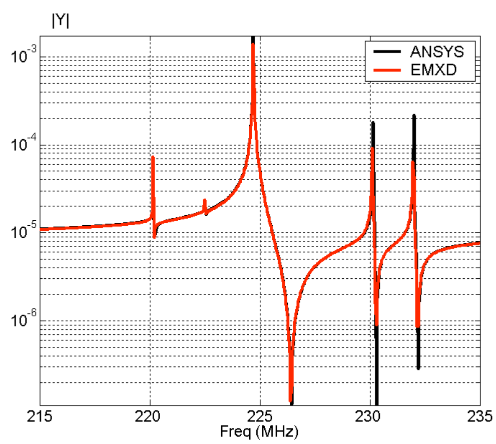

Figure 6. ANSYS-EMXD results comparison

B. Suspended resonator 3D simulation

After this validation, we analyzed the suspended resonator structure presented in Fig. 7 with EMXD. The structure is clamped on lateral sides (no mechanical displacement in space directions), the bottom electrode is grounded and a potential constraint is applied to the top electrode.

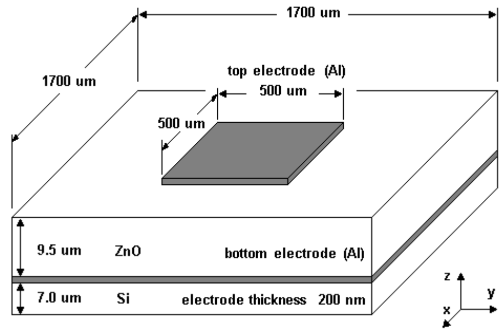

Figure 7. Suspended resonator 3D structure [2]

We obtained curves plotted on Fig. 8.

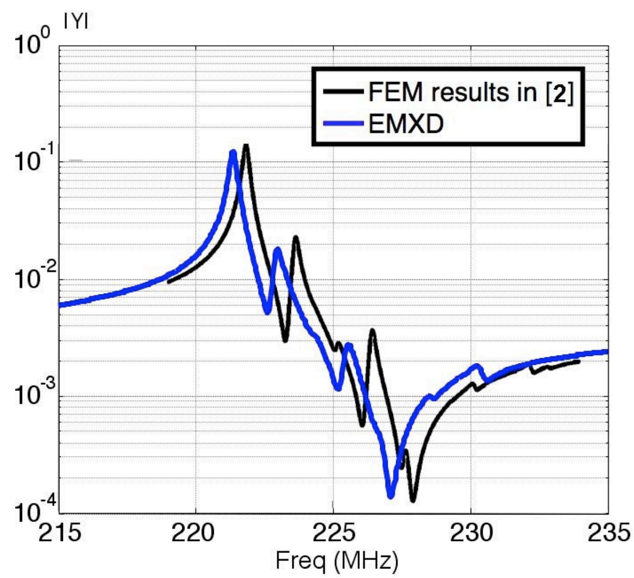

Figure 8. Suspended resonator electrical admittance

On Fig. 8, electrical admittance modulus variations are plotted. The black curve has been taken from [2] and the blue curve has been obtained with EMXD. Because any material mechanical constants or losses are given in [2] and since we considered literature datas, we obtained a little frequency shift and a stronger attenuation for some frequency.

But, the most important thing is that the admittance computed using 3D FEM software shows spurious resonance between resonant and antiresonant frequencies. In order to attenuate or suppress those spurious resonances, we need to identify their physical origin.

C. Mechanical displacement modes display

In order to identify spurious modes, we have plotted the mechanical displacement for four modes (Fig. 9).

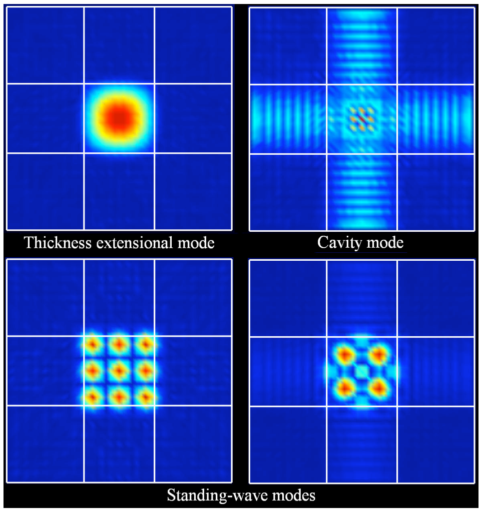

Figure 9. Suspended resonator mode shapes at resonant frequencies

The first mode is the so-called thickness extensional mode. It corresponds to the maximum energy coupling and to minimum mechanical losses. This mode is the one taken into account in 1D analytical model.

The second mode is a cavity mode. Its origin is the artificial boundary conditions considered on structure edges. Domain truncation causes reflection of the wave on clamped lateral sides. Then a standing wave may appear at certain frequencies. Those modes are modeling errors and may be suppressed by considering material losses or by using absorbent conditions or acoustic perfectly matched layers (PML).

Standing wave modes are harmonic thickness extensional modes due to acoustic wave reflection on top electrode edges. They appear as spurious modes in the electrical response. In order to use this electrical response for oscillator or filter applications, we need to suppress those modes. Different solutions can be considered.

D. Spurious modes suppression methods

1) Apodization method

The first solution consists in “cutting“ a triangular part of the square top electrode and “pasting” it on another edge (Fig.10). Then we obtain a quadrilateral electrode with no parallel sides.

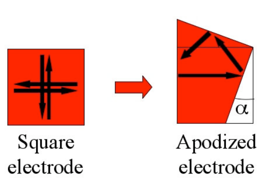

Figure 10. Apodization applied to a square electrode

Standing waves cannot appear since multiple reflections are not constructive. We can notice on Fig.11 that spurious modes are not or weakly coupled as the apodization angle increase. Our 3D simulation software permits to analyze an entire apodized resonator and will be very useful in this case for determining an optimum apodization angle.

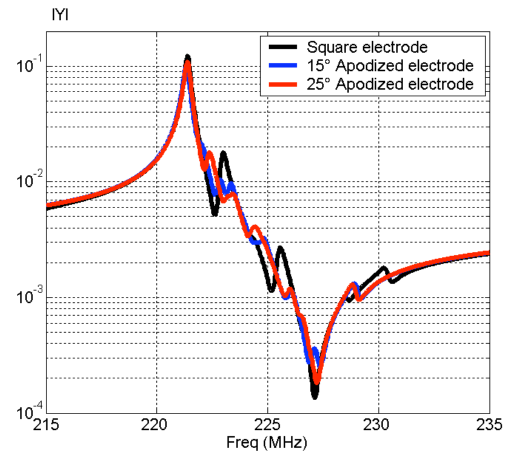

Figure 11. Apodized top electrode electrical admittance for two apodization angle values

2) Edge loading method

We then considered another solution proposed in [3]. A narrow region is deposited at the edge of the suspended resonator top electrode (Fig. 12). This thickened region constitutes a frame that matches the acoustic impedance and suppresses reflection on top electrode edges. Within certain optimum range for the edge region width, the resonator operates in a mode where the mechanical displacement is constant on the top electrode surface (Fig. 13).

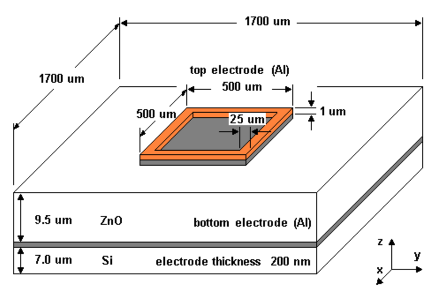

Figure 12. Framed top electrode suspended resonator 3D structure

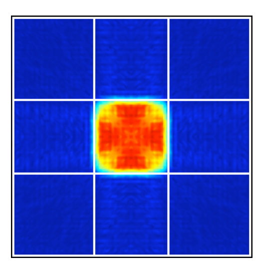

Figure 13. Framed top electrode suspended resonator thickness extensional mode

It can be observed that the electrical response is spurious modes free (Fig. 14). Standing waves on top electrode are not coupled. Moreover, 3D resonant frequency tends toward 1D result.

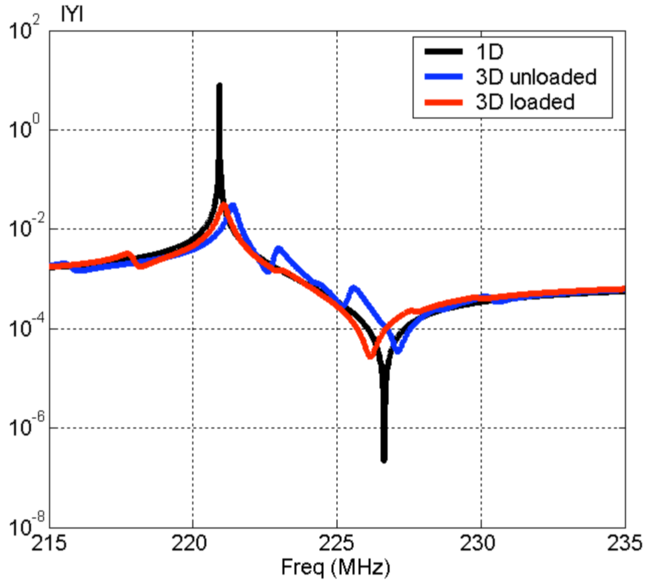

Figure 14. Framed top electrode suspended resonator admittance

V. CONCLUSION

A 1D analytical and a 3D FEM based simulation tools developed at Xlim and first 3D FEM results of BAW resonator structures have been presented. The 1D model permits to quickly design resonator stacks by determining layer thickness that correspond to the objective resonant frequency. 3D FEM model is a powerful tool to predict spurious modes that may appear in transverse directions. It mostly allows solution development of more complex structures to attenuate or suppress spurious modes from the electrical response. It may also allow designing spurious mode free structures.

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