Study on the Performances of AlScN based SAW/BAW Hybrid Resonators

A Parametric Analysis of Acoustic Wave Resonators with Large Figure of Merit

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***Abstract*—In this study, we analyze a 3rd type of FBAR's fundamental mode by finite element method. We show the importance of the substrate's wave velocity and conductivity on the electromechanical coupling efficiency. Then we demonstrate that etching traditional SAW sensors in between its electrodes is an effective solution to increase its performances. Finally, the finite device simulations of optimized geometries demonstrate the full potential of AlSc(0.4)N based SAW/BAW hybrid resonators: an impedance response free of spurious modes and large figure of merit ($k_{t\ FD,1.35GHz}^2 = 23.48\%$).**

Keywords— AlN, AlScN, SAW, BAW, hybrid resonators, parametric study, harsh environment operations, piezoelectricity, FEM, COMSOL Multiphysics

I. Introduction

The thermal behavior of Aluminum Nitride (AlN) makes it very interesting for operations at high temperature. Significant advances in Scandium doped AlN have been made thereby improving electromechanical coupling of Contour Mode Resonators (CMRs) and Bulk Acoustic Wave (BAW) resonators [1-4]. However, even if doping AlN with Scandium (Sc) increases its piezoelectric coefficients, the recorded electromechanical coupling factor (k_t^2) of traditional Aluminum Scandium Nitride (AlScN) Surface Acoustic Wave (SAW) resonators only reaches 1% to 5%[5-7].

A 3rd type of FBAR has been introduced in 2013 by Plessky et al. [8]. This hybrid resonator is manufactured by etching the piezoelectric material in-between the electrodes of a SAW structure (see.Fig.1). Compared with traditional SAW resonators, this geometry has demonstrated an enhanced electromechanical coupling factor when used within d33 driven piezoelectric materials such as AlScN. Furthermore, thanks to their high resonance frequency (f_{res}) tunability and high electromechanical coupling efficiency, 3rd type of FBARs exhibit a great potential for multi-GHz filtering.

Hashimoto and al. [5] have shown that substrates with high wave velocity promote the energy's confinement in the piezoelectric layer and hence increases the performances of SAW resonators.

This study aims to lay the background for future development and optimization of AlSc(0.4)N SAW/BAW hybrid resonators for harsh environment operations. Therefore, we investigate the behavior of the 3rd type of FBAR's fundamental mode by finite element method using COMSOL Multiphysics. The schematic of the simulated model is shown in Fig. 1.

Then we run a parametric analysis to demonstrates the relation between the geometry and the performances. We show a direct relation between the etching depth and k_t^2 (the deeper the better). We also find the optimal thickness-to-pitch ratio is not constant but switch from 0.4 (as demonstrated for traditional SAW) up to 0.7 for a 90% etch of the piezoelectric layer.

Finally, we select sub-optimal designs and run finite device simulations to confirm our previous studies and compute their effective Figure of Merit (FoM). The performances between the periodic cell and finite device simulations are quite similar: we only record small variations with $k_{t,periodic}^2 = 23.72\%$ & $k_{t,finite}^2 = 23.48\%$.

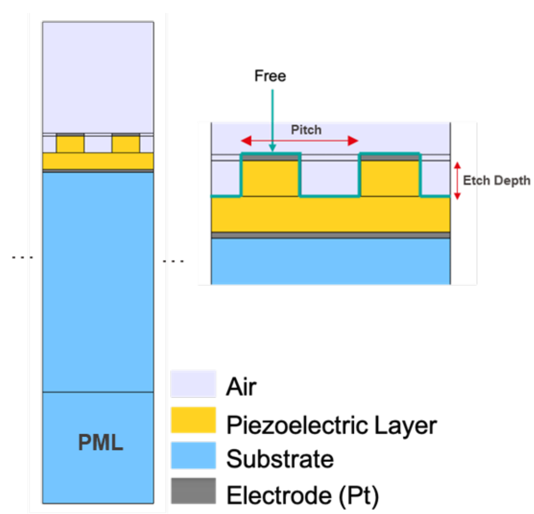

Fig 1: Schematic of unit cell of AlSc(0.40)N hybrid resonator.

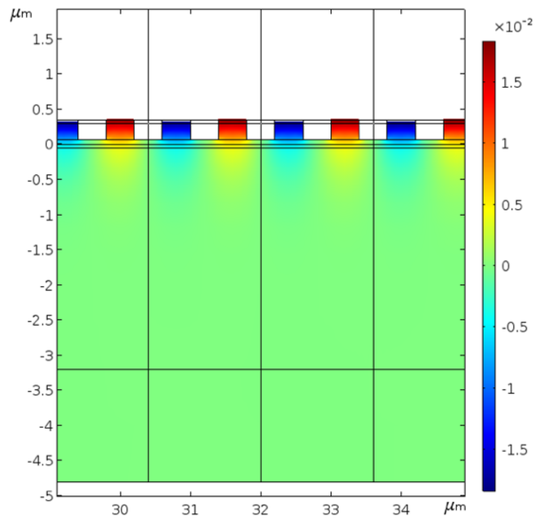

Fig 2: Representation of the vertical displacement of a finite AlSc(0.40)N hybrid resonator. Simulation parameters: pitch = 1.0 [µm]; etching depth = 75[%]; coverage = 50 [%]; tAlN = 0.3 [µm]; tP t = 50 [nm]; Substrate=SiC ; Scale factor = 1.

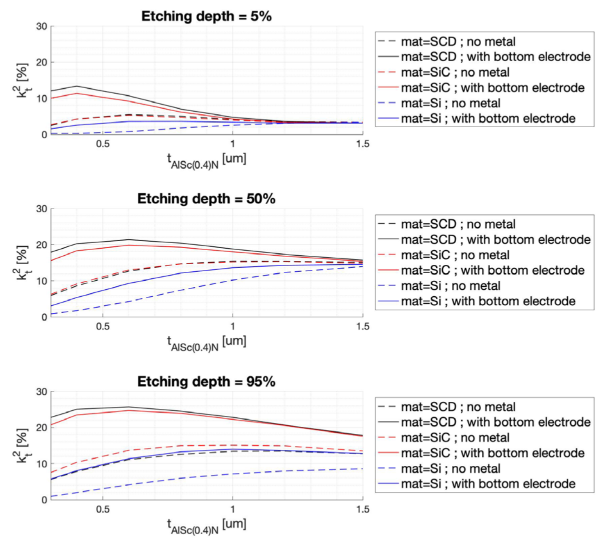

Fig 3: Impact of the substrate and bottom electrode onto electro-mechanical coupling (kt2) in function of AlSc(0.4)N thickness. Simulation parameters: pitch = 1.0 [µm]; tPt = 50 [nm]; coverage = 50 [%]; Substrate=SiC

II. METHODS

A. Periodic Cell Substrate's Material Analysis

We first extended the study of Hashimoto et al to see how the substrate's material impact the performance of 3rd type of FBAR. The results are alike a traditional SAW resonator. Indeed, k_t^2 increases within the wave velocity in the substrate.

In this first section, we extend their analysis to 3rd type FBARs.

We compared the performances of a set of design with three different substrate's materials: Single Crystal Diamond (SCD), Silicon Carbide (SiC) and Silicon (Si). The Fig. 3 presents the variation of the electro-mechanical coupling factor with the thickness of the piezoelectric layer in the presence of a bottom electrode.

The electro-mechanical coupling factor is computed using the following formula:

$$k_t^2 = \frac{\pi^2}{4} \frac{f_s \cdot (f_p - f_s)}{f_p^2} \qquad (1)$$

where f_s and f_p are the series and parallel resonant frequencies respectively.

As we expected, the coupling efficiency is much higher for SCD and SiC than for Si. Indeed, the speed velocity of these materials is high, and their isotropic damping factor are lower than Si at the GHz range. Since we planned to manufacture our devices, we decided to select a SiC substrate which is widely available, beside the slightly higher efficiency of SCD.

B. Periodic Cell Parametric Analysis

The substate being selected, we determine in this section the relation between geometry and performances. We run a total of 450 simulations to create a complete set of designs with the parameter's values given in TABLE I.

TABLE I. PARAMETERS VALUES USED DURING THE PERIODIC CELL PARAMETRIC STUDY

Parameters	Unit	Value
pitch	um	[0.8; 1.0; 1.2; 1.4; 1.6]
etching depth	%[a]	[5; 25; 50; 75; 95]
piezoelectric layer's thickness	um	[0.3; 0.4; 0.6; 0.8; 1.0; 1.5]
electrode's thickness	nm	[50; 75; 100]

[a] Relative to piezoelectric layer's thickness

1) Impact on Performances

As expected, the performances of 3rd type FBARs highly depends on the etching depth. We recorded a 265% increase of $\max(k_t^2)$ while swiping the etching depth from 5 to 95%.

Unlike the predictions of Paschenko and al.[9], the optimal thickness-over-pitch ratio that maximize k_t^2 is not constant. In Fig. 4, we plotted k_t^2 in function of this ratio and computed 6th order polynomial approximations. For small etching values, our result ($r_{opt\downarrow} = 0.41\,[-]$) matches the similar study conducted by Hao and al. [10] on SAW devices. However, this optimal ratio increases to $r_{opt\uparrow} = 0.7 \pm 0.05\,[-]$ for higher etching depths (> 50%).

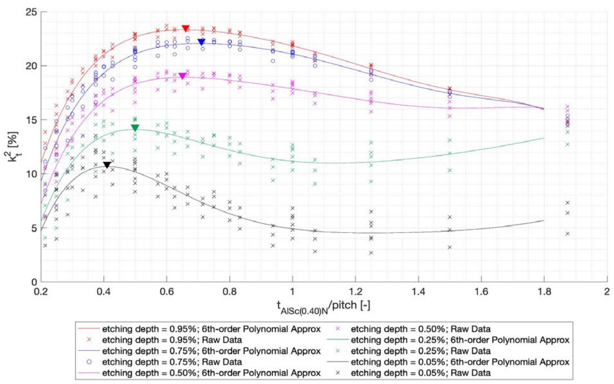

Fig 4: Evolution of the optimal thickness to pitch ratio in function of the etching depth for AlSc(0.4)N hybrid resonator on a SiC substrate. Results of a parametric simulation with a constant coverage of 50%. The filled triangles represent the maximal value of the peaks of the approximation curves.

2) *SAW or BAW Mode ?*

Knowing the acoustic wave's velocity in the piezoelectric layer, a good approximation of the resonance frequency is defined for SAW and BAW resonators which are pitch and thickness dependent respectively. In the introduction of their 2017 paper, Paschenko et al. describe the 3rd type FBARs as an array of BAW sensors that excites a SAW in the non-piezoelectric substrate [11]. However, we found that both the pitch and the piezo-electric layer's thickness have an impact on the resonance frequency (see Fig.5). Therefore, a two dimensional cavity modes exists where the respective dominances of SAW or BAW mode are driven by the etching depth.

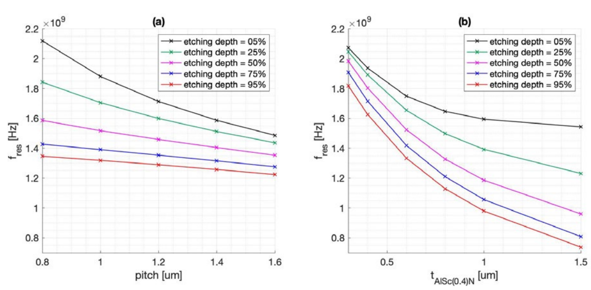

Fig 5: Impact of the pitch (a) and piezoelectric layer thickness (b) onto the resonance frequency of a AlSc(0.4)N hybrid resonator for different etching depth.

C. *Results Validation*

To validate our parametric study, we decided to compare our results with a finite device simulation. The device is composed of a total of 50 pairs of electrodes surrounded from both sides with a λ/2 reflector (composed of 20 shorted electrodes). The Fig. 2 is a representation of the vertical displacement at the center of the device at resonance frequency.

TABLE II. PARAMETERS VALUES USED DURING THE PERIODIC CELL PARAMETRIC STUDY

Simulation	**Design**	f_p **[GHz]**	f_s **[GHz]**	k_t^2 **[%]**
Periodic Cell	Optimal[b]	1.358	1.522	23.72
	Frequency Tuned[b]	2.417	2638	18.91
Finite Device	Optimal[b]	1.359	1.521	23.48
	Frequency Tuned[b]	2.418	2.635	18.65

b. Pitch. = 1.0um, etching depth = 95%, piezoelectric layer's thickness=0.6um, electrode's thickness=75nm

c. Pitch. = 0.8um, etching depth = 75%, piezoelectric layer's thickness=0.3um, electrode's thickness=50nm

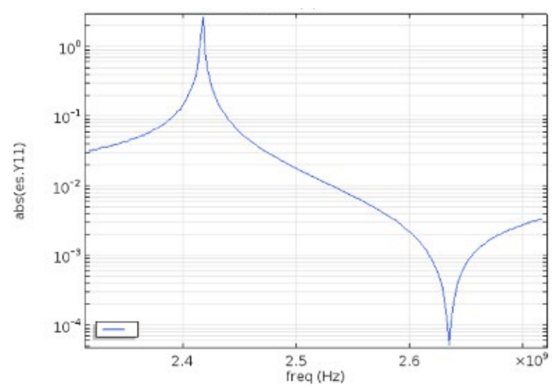

Fig 6: Representation of terminal's impedance of a finite AlSc(0.40)N hybrid resonator from the FD simulation. Simulation parameters: pitch=0.8 [µm]; etching depth = 75[%]; coverage = 50 [%]; tAlSc(0.4)N=0.3[µm]; tPt = 50 [nm]; Substrate=SiC.

We run the finite device simulation for 2 designs:

- The geometry that exhibits the best k_t^2 score during the parametric study. This "optimal design" is used to give a performance baseline for SAW/BAW hybrid resonators.
- The geometry with the maximum k_t^2 score within the 2.0-2.5GHz bandwidth. This design is used to operate in the multi-GHz range.

The TABLE II. compare the resonance frequencies and k_t^2 of both simulations. The variations of f_p and k_t^2 are negligible (0.11% and 1.4% respectively) and confirm the validity of our previous study.

Furthermore, the impendence response is free of any spurious modes (see Fig. 6) which makes our hybrid SAW/BAW resonator well adapted to filtering in the GHz bandwidth.

III. CONCLUSIONS

After the highlight of a correlation between substrate's acoustic wave's velocity and electromechanical coupling efficiency, a parametric study has shown the potential of SAW/BAW hybrids design. This analysis has demonstrated an important increase of performance by increasing the etching depth. It also enabled us to build a data base allowing a further modelling of underlying mechanisms. With new records in the literature, we noticed a shift in the optimal thickness-over-pitch ratio while the etching of the piezoelectric layer is increase. We introduced a coupling between a SAW and a BAW in 3rd type FBARs to explain the dependence of the resonance within the pitch and piezoelectric layer's thickness. Finally, two selected designs have been studied further with a finite device simulation. Through this study, we have validated the performances of these designs and the validity of our work.

With a higher electromechanical coupling factor than SAW resonators SAW/BAW hybrid resonators display the highest FoM ever recorded for AlScN based resonators with k_{t}^{2} reaching 23.48%. Thanks to its performances and high frequency capabilities, SAW/BAW hybrid resonators are a high-potential candidate for a wide range of applications such as high frequency filters and sensing in harsh environment.

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