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LiNbO₃ Film Bulk Acoustic Resonator

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Abstract— As layer transfer techniques have been notably improved these passed years, lithium niobate (LiNbO₃) appears as a candidate for the next generation of ultra wide band RadioFrequency (RF) filters. Depending on the crystalline orientation, LiNbO₃ can achieve electromechanical coupling factors Kt² more than 6 times larger than those of sputtered aluminium nitride films. In this paper, a process based on direct bonding, grinding, polishing and Deep Reactive Ion Etching (DRIE) is proposed to fabricate a single crystal LiNbO₃ Film Bulk Acoustic Resonator (FBAR). From the fabricated test vehicles K₁² of 45% is measured confirming the values predicted by theoretical computations.

I. INTRODUCTION

RF passband filters are required in telecommunication systems to select the working band of the RF signal. In that purpose, piezoelectric materials are used to develop passive solutions such as Surface Acoustic Wave (SAW) filters or Bulk Acoustic Wave (BAW) filters which for years have satisfied mobile phone standards. Among theses acousticwave-based filters, one operating mode is particularly used due to its design simplicity and adaptability, based on impedance element association as for the so-called ladder structure for instance. In that specific case, two kinds of resonators are connected, one having its parallel resonance corresponding to the series resonance of the other one. The bandwidth of the filter is proportional to the frequency spacing between series and parallel resonances, respectively f_s and f_p of one of these resonators. For a BAW configuration, where AC polarization is applied between the two faces of the layer, this spacing is linked to the electromechanical coupling factor K_t^2 by equation (1):

$$k_t^2 = \frac{\pi}{2} \frac{f_s}{f_p} \frac{1}{\tan\left(\frac{\pi}{2} \frac{f_s}{f_p}\right)}$$
(1)

For the next generations of ultra wide band RF filters for which relative bandwidth in excess of 10% and drastic loss

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requirements (less than 3 dB within the passband) are mandatory, no immediate solutions emerge. Indeed SAW filters are still limited by their power handling capability [1]. For BAW devices, the only efficient filters are already commercialized and based on sputtered Aluminium Nitride. In spite of suitable quality factors for telecom applications, AlN is not suited for ultra wide band as its intrinsic coupling factor K_t^2 is limited to 7.5% [1,2]. An alternative to AlN would be ZnO based resonators; however they do not exhibit higher values for either K_t^2 or Q factor [2]. To overcome the coupling factor problem, sputtered or sol gel depositions of lead-zirconate-titanate (PZT) and lead-manganese-niobium-titanate (PMNT) have been investigated despite the major issue of limited Q factors due to relaxation of ferroelastic domain walls at the GigaHertz range [2,3].

The solution consisting in the use of single crystal materials such as LiTaO₃ or LiNbO₃ for reaching larger K_t^2 and Q factors is particularly regarded here. These materials are extensively used for the manufacture of SAW filters. Both materials exhibit large electromechanical coupling coefficients and excellent quality factors, clearly larger than those of sputtered piezoelectric films for BAW resonators as their frequency/quality factor products largely overcome 10^{13} whereas sputtered film-based solution rarely reach this value. Moreover, in BAW configuration these two materials can exhibit electromechanical coupling factors up to 45% (for LiNbO₃), i.e. more than twice those of SAW devices.

Since the 70's, layer transfer appears to be a promising method to obtain pure single crystal thin films [4]. Grinding-polishing [5,6] and the more advanced technique of ionic implantation [7,8,9] have proven the advantage of the extra freedom for the choice of crystalline orientations and thus the choice for acoustic waves, coupling factors or temperature coefficient of frequency (TCF).

Comparing the single crystal acoustic properties to those of sputtered thin films, one can wonder that the use of thinned single crystal layers in place of deposited AlN films in RF filters should yield notable increase in coupling and quality factors, as single materials should noticeably be less affected by structural defects due to the film fabrication process (grains, columns, cracks and orientation defects) which generates physical dispersion and hence acoustic losses. These advantages more than compensate the difficulties of the single crystal thin film transfer process.

II. EXPERIMENTAL PROCESS

The aim in this paper is to prove the feasibility of single crystal lithium niobate FBAR. Although standard FBAR applications need frequencies above the GigaHertz, we will in this paper discuss direct wafer bonding and grinding-polishing of X-cut LiNbO₃ down to 6.6 microns, corresponding to a resonant frequency near 250 MHz. A final single crystal LiNbO₃ Film Bulk Acoustic Resonators is obtained with very large electromechanical coupling factor K_i².

In order to validate such a process, two different wafers are involved. A 100mm wafer of X-cut lithium niobate, further considered as donor or "D" is used for the two shear waves electromechanically coupled in BAW configuration. A second double-side polished Si wafer is used, further considered as handling or "H" wafer (Fig. 1).

After substrate cleaning, a metallic electrode AlCu (100 nm) layer and a silicon oxide layer are deposited on the donor wafer. Another layer of SiO₂ (200 nm) is also deposited onto the handling wafer and then, the surfaces are cleaned and prepared for room-temperature hydrophilic bonding. On both H and D wafers, surface roughness is controlled to be less than 5 Å rms as measured by AFM $1x1\mu$ m². Then a direct bonding of H and D wafers is performed at the two silicon dioxide surfaces. Grinding followed by polishing of the rear face of lithium niobate ("D" wafer) is achieved with a careful control of process parameters. An aluminium (100 nm) top electrode is finally deposited and 2 port resonator patterns are obtained via an ion beam milling technique.



Figure 1. Experimental process for LiNbO3 layer transfer technique

III. HBAR MEASUREMENTS

At this step the device is a High overtone Bulk Acoustic Resonator and has been electrically characterized with a Vector Network Analyzer with a SOLT calibration procedure. In HBAR, although the thinned piezoelectric layer acts as transducer, the acoustic wave mainly propagates into the substrate. The resulting measurement is a set of peaks corresponding to the high order harmonics of the thickness resonance of the substrate, modulated by the behaviour of the thinned piezoelectrically active layer. This modulation corresponds to the response of an equivalent thinned layer transducer on a semi-infinite substrate. Transduction efficiency is evaluated across the electromechanical coupling factor Kt² of the thinned piezoelectric layer and is obtained from Fig.2 with equation (1). In this HBAR, K_t^2 of the thinned piezoelectric film can be evaluated considering the modulation of the LiNbO₃ X-cut resonator multi-mode response. Along that approach, K_t^2 is found to reach a top value of 45% (Fig.2) which is more than 6 times larger than AlN theoretical value of 7%. For acoustic wide band filtering solutions, submicron thick monolithic layers of lithium niobate would be required, possibly obtained by the Smart Cut $^{\rm TM}$ technology to solve both homogeneity and reduced thickness matters [10].



Figure 2. High order harmonics of the HBAR modulated by the first two harmonics of the thinned LiNbO₃ layer. From the modulation of the thin piezoelectric layer f_s and f_p are the extracted series and parallel resonances of this thin layer. Inset is a schematic view of LiNbO₃ HBAR.

IV. FBAR MEASUREMENTS

A final Deep Reactive Ion Etching (DRIE) step using the Bosch process enables the etching of the rear face of Si "H" wafer (550 μ m) with the SiO₂ as an etch-stop layer. Hence the remaining resonator stack is composed as follows: Al (100 nm) / X-cut LiNbO₃ (6.6 μ m) / AlCu (100 nm) / SiO₂ (400 nm). This Film Bulk Acoustic Resonator (FBAR) is tested along the same procedure as for the previous HBAR. Fig.3 shows the first two harmonics and this time a K_t² of 43% is directly extracted from these measurements via equation (1).



Figure 3. Fundamental and 3rd harmonics of the pure shear mode of the self-supported thinned X-cut LiNbO₃ plate. A K_t² close to 45% is measured. Inset is a schematic view of LiNbO₃ FBAR.

For further understanding of this resonator, we use simulations based on the scattering matrix method [11]. This method includes a Fahmy/Adler formulation [12], which describes vibrations of multilayered structures as the linear superposition of plane waves propagating in each layer. Electromechanical fields are then calculated from the applied boundary conditions (stress-free surfaces, continuity at the interface between two materials, and electrical excitation), which allows to determine the surface electrical charge density at the interface between the excitation electrode and the piezoelectric material and from this the electrical admittance or impedance. Fig.4 shows the corroboration of the large value obtained experimentally (in black) and from simulations based on the scattering matrix method (in black). Similarly one can calculate from the material constants the theoretical value of 45%, close to the experimental value of 43%.



Figure 4. Comparison of the first resonance of a FBAR response simulated considering a homogeneous thickness on the LiNbO₃ (black), assuming an inhomogeneous thickness of the LiNbO₃ plate simulated by 20 resonators connected in parallel (red), and compared to the experimental admittance of the resonator (blue).

Beyond the large electromechanical coupling factor measured, the consistency between the HBAR extraction and FBAR

measurements is of great interest: a rather good approximation of this value is easily obtained with HBAR.

V. EXPLAINING THE QUALITY FACTOR

However, it is worth noting that the tested resonators did exhibit quite poor quality factors (in the vicinity of 64). The origin of this disappointing result is due to the thickness homogeneity degradation while performing the grinding operation. From surface profiler measurements, we observed a linear thickness difference of 100 nm across the 150 μ m width of the active area of the tested resonators. As frequency is inversely proportional to the thickness and quality factor is extracted from the full width at half maximum of conductance peaks, even for a non lossy material a 100 nm shift in thickness is the limiting effect concerning the quality factor.

Indeed, we can write for the first mode with the approximation:

$$FWHM \approx f_r(e) - f_r(e + \Delta e) = \frac{v}{2e} - \frac{v}{2(e + \Delta e)}$$
(2)

$$FWHM \approx \frac{2v.\Delta e}{4e.(e+\Delta e)}$$
(3)

$$Q = \frac{f_r}{FWHM} = \frac{v}{2.e} \cdot \frac{4e(e + \Delta e)}{2v \cdot \Delta e} = \frac{e + \Delta e}{\Delta e}$$
(4)

Where $f_r(e+\Delta e)$ and $f_r(e)$ are the resonant frequencies of a resonator respectively with the maximum thickness $e+\Delta e$ and minimum thickness e. Q is the quality factor and v the velocity of the acoustic wave considered. Numerically, for the 6.6 micron thickness e of our FBAR and with $\Delta e=100$ nm, Q is limited to 67. The same calculation based on an optical interferometer measurement of surface roughness of 0.6nm RMS - $ie \Delta e = 1.2$ nm - would lead to a maximum Q of 5500, comforting the idea that the limiting effect is the inhomogeneous thickness.

Based on the scattering matrix method, simulations are performed with 20 parallel resonators – LiNbO₃ material Q is set above 10000 – with thicknesses distributed from 6.55µm to 6.65µm, providing a good approximation of the actual FBAR (in red). The result is in good agreement with the previous explanation as shown in Fig.4. A broader peak on the resonator conductance is observed leading to a poorer quality factor, as experimentally observed. Matching with experimental data is performed reinforcing the hypothesis of linear thickness increase. Two other phenomena are observed in Fig. 2:

- The fast 2nd shear wave appears between series and parallel resonance of the slow shear wave with larger k_t² than what is experimentally observed.
- Oscillations around the resonance peak and for frequencies higher than the antiresonance peak are HBAR behaviour due to the design of our two ports resonators.

Finally, we can take into account the material properties extracted from simulations to show what would be a typical acoustic wide band filter in the GigaHertz range. Fig. 5 is a comparison between a standard GSM band pass filter based on Solidly Mounted AlN Resonators and a possible ultra wide band filter based on LiNbO₃ FBAR. More than 6 times larger bandwidth is observed.



Figure 5. Comparison of non optimized simulated pass band filters based on X-cut LiNbO₃ (black) and traditional sputtered AlN (red). The simulations are performed with the scattering matrix method. The stacks of AlN and

LiNbO₃ band pass filters are designed so as to provide centre frequency close to 2 GHz.

CONCLUSIONS

In this paper, a 6.6 μ m single crystal X-LiNbO₃ FBAR has been fabricated by wafer bonding, grinding polishing and deep reactive ion etching. A K_t² value as high as 43% is demonstrated and compared to theoretical and simulated values. However, it has been shown that controlling accurately the thinned layer thickness reveals to be a key-parameter for reaching high Q factor resonances. Larger quality factors as well as thinner layers might be achieved by improvement of the process or more advanced techniques such as Smart CutTM in order to obtain sub micron single crystal piezoelectric layers [10] and hence the feasibility of ultra wide band RF filters.

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