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Design and characterization of high-Q SAW resonators based on the AlN/Sapphire structure intended for high-temperature wireless sensor applications

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Abstract—Aluminium nitride piezoelectric thin films grown on sapphire are strong candidates for high-temperature surface acoustic wave (SAW) sensors, due to their thermal stability, large bandgap, high acoustic velocity and suitable electromechanical coupling. However, thin-film resonators need more design efforts than those based on bulk crystals, due to the usually limited thickness of the piezoelectric films, and to acoustic properties disparities between the latter and their host substrate. This work presents an optimization of AlN/Sapphire-based SAW resonators with high quality factors for high-temperature applications. It combines specifically grown, 3 μm -thick aluminium nitride films, with the use of aluminium electrodes for their low density and resistivity, as an alternative to heavier electrodes like Pt. These electrodes allow for much lower mechanical losses and higher quality factors, in spite of needing passivation for increased lifetime. A standard resonator design is first presented and used for preliminary tests, in order to monitor the AlN/Sapphire structure with unprotected aluminium electrodes, for temperatures up to 600°C. A quasi-synchronous, optimized design is then proposed for higher quality factors and wireless sensing compliance. The high temperature characterizations confirmed that much larger quality factors can be retrieved from this optimized design. The quasi-synchronous resonators proposed in this study remain well-tuned for temperatures up to 400°C, and show high quality factors, as high as 3400 at 400°C.

Index Terms—Sensors, Surface acoustic waves, Resonators, Aluminium nitride, High temperature.

I. INTRODUCTION

SURFACE acoustic wave (SAW) devices have been strongly promoted for their sensing capabilities on a wide range of physical quantities [1]. This includes – among others – temperature, pressure, and strain sensors, that are naturally compatible with batteryless and wireless operation, making this technology particularly suitable for high-temperature

applications. However, the availability of piezoelectric materials with good physico-chemical stability proves to be crucial in this context. The usual SAW substrates such as quartz and congruent lithium niobate are not considered as suitable for high-temperature operation above 400°C [2,3]. So far, langasite ($\text{La}_3\text{Ga}_5\text{SiO}_{14}$; LGS) remains the only bulk material whose stability in air atmosphere has been demonstrated for long lifetimes, up to 1000°C [4]. However, its relatively low SAW velocity (2500-3000 $\text{m}\cdot\text{s}^{-1}$) and high acoustic propagation losses are drawbacks for high frequencies, while its electrical resistivity drops with temperature due to oxygen ion transport and diffusion in the lattice, making it difficult to design resonators operable above 700°C [5]. In the last decade, aluminum nitride (AlN) piezoelectric thin films grown on sapphire substrates have been proved to be strong candidates as an alternative to LGS for high-temperature SAW applications due to their thermal and chemical stability up to more than 1000°C [6-8]. This bilayer structure offers moderate electromechanical coupling coefficient, comparable to that of LGS crystals (0.3-0.4% at best), suitable for the achievement of SAW resonators. On the other hand, the AlN/Sapphire structure is compatible with high-frequency applications due to its large acoustic velocity (around 5500 m/s). Its main advantage for the intended application is likely the huge bandgap of AlN (6.2 eV) which results in outstanding dielectric properties at high temperatures up to 1000°C and more [5]. The suitability of the AlN/Sapphire bilayer structure for high-frequency high-temperature SAW applications has thus been established. However, several challenges remain to be faced before commercializing SAW sensors based on this structure. In particular, SAW resonators with quality factors of several thousands, compatible with wireless interrogation, are highly needed. Thin-film, layered, resonators need more design efforts than those based on bulk crystals. It is also necessary to pay

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attention to the evolution of the Q-factor of the resonators with the temperature. This evolution has not been reported so far. Therefore, this work presents an optimization of AlN/Sapphire based SAW resonators for high quality factors (Q) and the evolution of this parameter with temperature, up to 400°C.

II. CONSIDERATIONS ON RESONATOR DESIGN AND OPTIMIZATION

This study focuses on the 433 MHz and 868 MHz industrial, scientific and medical (ISM) bands : the typical wavelengths associated to these operation frequencies are respectively around 13 and 6.5 μm on the studied AlN/Sapphire structure. The modelling was performed on a custom FEM/BEM software, including harmonic admittance calculations, with no electrical or mechanical loss considered. An introduction to the techniques used in the software can be found in refs. [9-11].

Initial simulations have been performed in order to assess the performance of resonators as a function of electrode thickness for a variety of electrode materials showing different densities, including Pt and Al (Figure 1), as a function of metallization ratio and relative electrode thickness (h_{el}/λ). The use of high-density electrode materials, like platinum or iridium-based alloys, leads to a strong decrease in the intrinsic

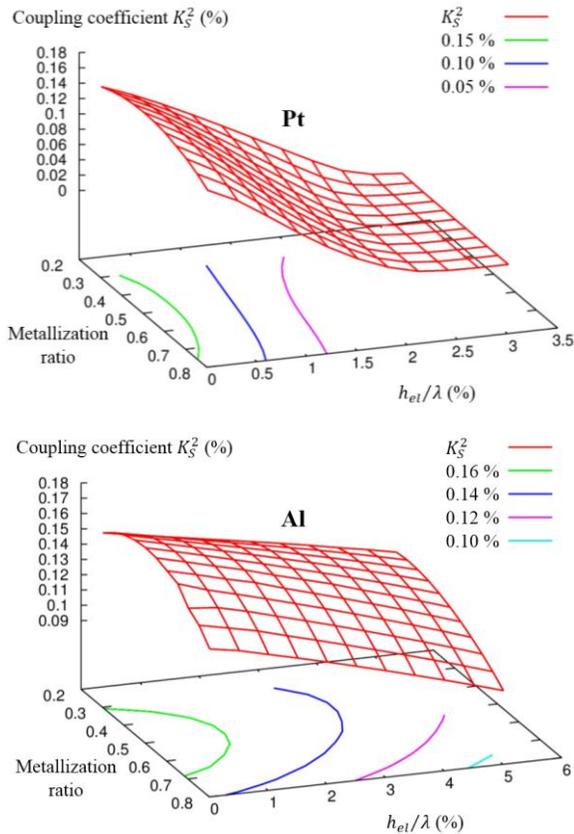


Fig. 1. Expected coupling coefficient for AlN/Sapphire structures under infinite electrode gratings (*top*: Pt, *left*: Al). Calculations made for an AlN thickness of 3 μm .

electromechanical coupling coefficient (K_S^2) of the substrate. Values of K_S^2 are typically twice lower for platinum than for lighter electrodes like aluminium, for an electrode relative

thickness of 1%, and nearly 20 times lower for $h_{el}/\lambda = 2\%$. Thus, in the case of Pt IDTs, K_S^2 is below 0.03% for an electrode relative thickness of 2%, and only 0.07% if this ratio is decreased to 1%. At the same time, the lower conductivity and higher mechanical damping in Pt will generally lead to lower Q compared to Al. Lower K_S^2 and Q would lead to low figures of merit: this would have a large negative impact on the wireless capabilities of such devices, reducing the interrogation distance to only some tens of centimeters at best. Moreover, the use of thinner Pt electrodes would intensify their coalescence encountered at high temperature, and thus obliterate the advantages of such electrode material.

Moreover, this study proposes to improve the quality factor by introducing a detuning between the interdigitated fingers (IDTs) and the reflectors, thus providing a quasi-synchronous resonator design. The resulting effective coupling coefficient is thus expected to decrease: this definitively invalidates the use of heavy electrodes for this application. Aluminium, on the contrary, shows a lower thermal stability compared to these heavy electrodes, but is still worthy of attention, especially when passivation or packaging can address its oxidation issues [12]. The choice of aluminium electrodes was then made for their low density and resistivity, as an alternative to heavier electrodes like Pt, in spite of their lower thermal stability.

In a first time, standard, synchronous resonators operating around the 433 MHz and 868 MHz (ISM) bands are investigated. Based on these characterizations, a quasi-synchronous, optimized design is then proposed for higher quality factors and wireless sensing compliance. Non-synchronous designs have been previously presented in the Literature for various resonator structures [13,14]. The slight detuning that results from non-synchronicity between the IDTs and reflectors, allows to reshape the resonance spectrum of the devices, and thus offers larger quality factors which is an essential parameter for the remote interrogation of SAW resonators.

The optimized AlN thickness was determined from the K_S^2 dispersion curves in order to keep a near-maximal electromechanical coupling at 433 MHz: it was chosen to be 3 μm . These modelling results are in good accordance with the studies previously reported in the Literature [15]. The targeted AlN thickness is beyond the usual thicknesses proposed by AlN films providers: a specific process has then been developed for the growth of thick AlN.

III. EXPERIMENTAL RESULTS

A. Substrate Preparation

The growth of 3 μm thick AlN substrates was performed on the basis of 25 nm thick AlN/Sapphire buffer templates wafers provided by Kyma Technologies, Raleigh, NC, USA, and based on an hydride vapor phase process. The piezoelectric layers were then deposited by DC magnetron sputtering (DCMS). Pinnacle™ Plus 5 KW with arc-suppression features was used. Power supply parameters and Deposition conditions were optimized to obtain efficient spark suppression. The use

of these low thickness AlN templates proved to offer a better crystalline quality, compared to the direct AlN deposition by DCMS on bare sapphire substrates. The deposition process was optimized in order to preserve the high crystalline quality of the AlN buffer layers for a thickness up to 3 μm , with near-epitaxial quality, leading to the expected structure for study: AlN (0001) / sapphire (0001) samples [16,17]. DCMS was chosen over metalorganic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) techniques [18], due its ability for strain management, which is crucial when it comes to achieve 3 μm thick layers. It was also preferred to high power impulse magnetron sputtering, because of the higher strains encountered with this latter sputtering technique [19,20]. In order to keep residual strain as low as possible, the pressure was set to 2.2 mTorr, and the power to 23 W/cm² of target. The deposition rate then reached 130 nm/min. The thickness of the deposited AlN layers was then determined by ellipsometry, following a Tauc-Lorentz model.

The synthesized AlN films are highly textured despite their large thickness, and show typical XRD FWHM rocking-curve values of 0.8° for the (002) reflex. This value remains close to the FWHM of the original 25 nm thick seed layer of AlN present on the templates, which was measured at 0.5°, as shown in Figure 2. It is also in good accordance with the properties of other thick AlN layers previously reported in the Literature by Martin *et al.* [21], who stated that the rocking curves tend to tighten with AlN thickness (reporting 1.14° for 2 μm thick films). This indicates an overall preservation of the AlN crystallinity throughout its deposition by DCMS, with a very limited rise of its mosaicity.

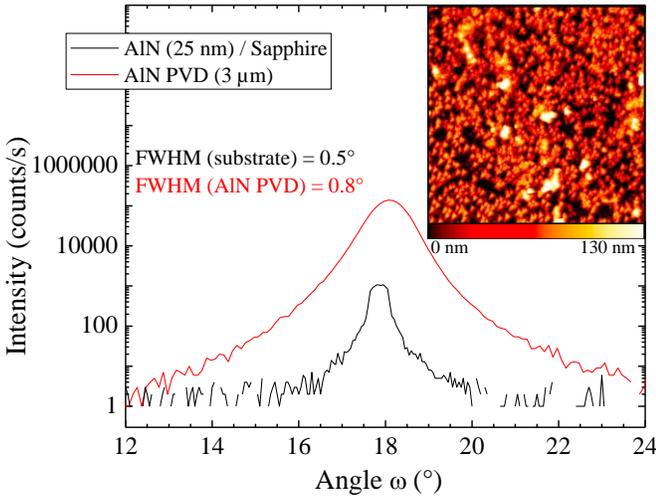


Fig. 2. XRD rocking curve of 3 μm thick AlN for (0002) peak, with respect to 25 nm AlN templates for comparison. Insert: AFM mapping of a $10 \times 10 \mu\text{m}^2$ of the same PVD grown AlN layer.

The resulting roughness of these 3- μm thick AlN layers was also measured by atomic force microscopy (AFM), leading to a typical RMS roughness of 30 nm (Figure 2: *insert*). However, this level of roughness did not interfere with the further processing of the AlN layers.

In addition, φ -mode XRD scans were used to study the epitaxial quality of the AlN films, as shown in Figure 3. These

give access to the in-plane texturing of the deposited layer. While the column twist of (10 $\bar{1}$ 1) planes was initially measured at 1.3° for the 25 nm thick AlN templates used in the study, the further deposition of 3 μm thick AlN led to a very limited overall column twist of 1.8°, demonstrating the quasi-epitaxial nature of the grown films.

B. Fabrication and Characterization of Standard Resonators

A first series of SAW devices was then fabricated on AlN/Sapphire substrates. The 200 nm-thick electrodes were deposited by DCMS. As mentioned hereinabove, the first series of devices, used to extract the material parameters for design optimization purposes, were based on synchronous resonators ($\lambda = 6.5 \mu\text{m}$, aperture = 40λ , 100 pairs, 2 x 200 reflectors). The IDT patterns were defined by UV lithography, and electrodes were etched using a mix of orthophosphoric and nitric acids.

The experimental tests were performed under air atmosphere, using an Agilent N5230A network analyzer and a RF probe station (S-1160, Signatone Corp., Gilroy, CA), equipped with a thermal probing system up to 600°C (S-1060, Signatone). The RF probes were adapted in order to withstand such high temperature measurements.

Thus, the resonance frequencies, Q factors and effective coupling coefficients could be extracted from the measurements of the resonators' admittances over this temperature range. Q was first obtained from the plotting of the real part of the resonator admittance Y_{11} , and expressed as the ratio, noted Q_Y ,

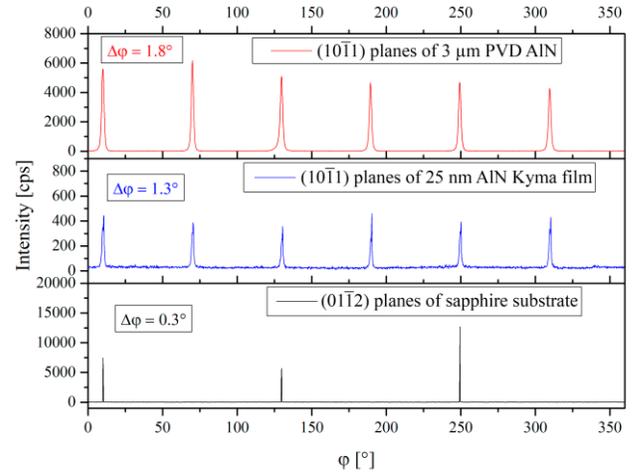


Fig. 3. X-ray diffractogram in φ -scan mode of 3- μm thick AlN obtained by PVD, and deposited on AlN Kyma (25 nm)/Sapphire.

of its peak frequency to its FWHM [18]. Another method was also applied for the optimized resonators, through the study of the phase shift occurring at the parallel (f_p) and series (f_s) resonance frequencies, as shown by the following formula proposed by Lakin [22,23]:

$$Q_{s,p} = \frac{f_{s,p}}{2} \left| \frac{d\varphi_Z}{df} \right|, \quad (1)$$

Where φ_Z is the phase of the impedance Z_{11} of the resonator. Both methods are accepted among others [20], as being as valid for the retrieval of Q . The Lakin method allows to dissociate the parallel and series quality factors, that are related to electrical and mechanical losses, according to the Butterworth-van Dyke (BVD) model.

The effective coupling coefficient was also determined with the following formula:

$$k_{eff}^2 = 1 - \frac{f_s^2}{f_p^2} \quad (2)$$

The characterizations of standard resonators ($\lambda = 6.5 \mu\text{m}$), show typical values of $Q = 325$ and $k_{eff}^2 = 0.56\%$ at room temperature (Figure 4), for a relative AlN thickness of 0.46.

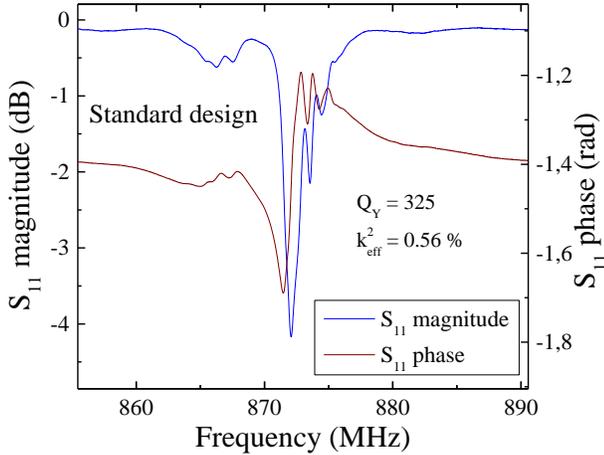


Fig. 4. Room temperature characterization of standard SAW resonators ($\lambda = 6.5 \mu\text{m}$), exhibiting spurious peaks in its return loss spectrum, and poor compatibility with wireless interrogation requirements., due to its low quality factor of 325.

The standard resonators performed very well in high temperature characterizations. Their frequency evolution up to 593°C has a slight curvature, with a first-order TCF of $-28 \text{ ppm}/^\circ\text{C}$, and a second-order TCF of $-36 \text{ ppb}/^\circ\text{C}^2$ (25°C being used as the reference temperature). This frequency behavior is in good accordance with previously published, experimental and calculated TCF results, for a relative AlN thickness around 0.46 [25]. The aluminium IDTs can still show enough stability in their electrical behavior up to 600°C . The Q factor of these standard resonators based on Al/AlN/Sapphire structure also remains almost constant, but at a value poorly compatible with wireless sensing, except at close distance.

C. Fabrication and Characterization of Optimized Resonators

The data extracted from the room temperature and high temperature characterizations of these standard resonators was then used to define a new, optimized resonator design, in order to reach higher Q factors, and thus better wireless sensing capabilities. The new design is based on a one-port quasi-

synchronous resonator design [26]. The geometrical parameters of the IDTs and of the reflectors were defined to keep the S_{11} peak frequency close to the higher limit of their frequency bandpass. The corresponding wavelengths were respectively equal to $\lambda_{IDT} = 12.64 \mu\text{m}$, and to $\lambda_{refl} = 12.57 \mu\text{m}$. The resonator design was then adjusted to maximize the electromechanical coupling through its parallel resonance frequency, which was positioned close to the impedance matching frequency of the resonator. The numerical evaluation of its quality factor is 8500.

This new resonator design was then process by UV lithography, using this time lift-off for the definition of the 200 nm thick aluminium electrodes.

Room temperature measurements were first performed on this series of optimized resonators. As expected, the optimized design shows a much better impedance matching, with return losses over -15 dB and Q values up to 8140, and a smaller k_{eff}^2 : 0.031%, as shown in Figure 5. The quality factor values were also retrieved from the impedance phase, for both parallel and series resonances. The series quality factor, illustrating mainly the mechanical losses, was calculated as $Q_s = 6380$, while the parallel quality factor, that also takes into account the electrical losses, was determined as $Q_p = 6300$.

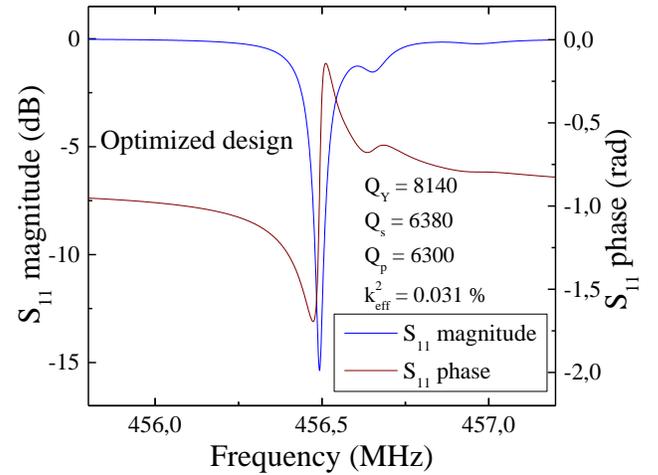


Fig. 5. Room temperature characterization of optimized quasi-synchronous SAW resonators ($\lambda_{IDT} = 12.64 \mu\text{m}$, $\lambda_{refl} = 12.57 \mu\text{m}$), exhibiting much better quality factor (8140) and cleaner S_{11} spectrum.

The resonators central frequency was noticed to be slightly shifted outside the 433 MHz band, which can be easily corrected through a new design. The figure of merit obtained by the product of Q and k_{eff}^2 is also improved by 38% through this optimization process, and also proves the usability of such structures for wireless operation [27].

The resonators were then individually characterized at higher temperature, and the RF signals – S_{11} and admittance magnitudes – were also retrieved for each temperature plateau, after complete stabilization of the chuck temperature. These spectra are much well defined than with the previously studied standard resonators. The admittance spectra extracted from high temperature characterizations (Figure 6) show clear

parallel and series resonance, in spite of a moderate increase of their impedance mismatch with temperature. A complete recovery of the signals happens during the cooling phase, as long as the temperature does not exceed 400°C.

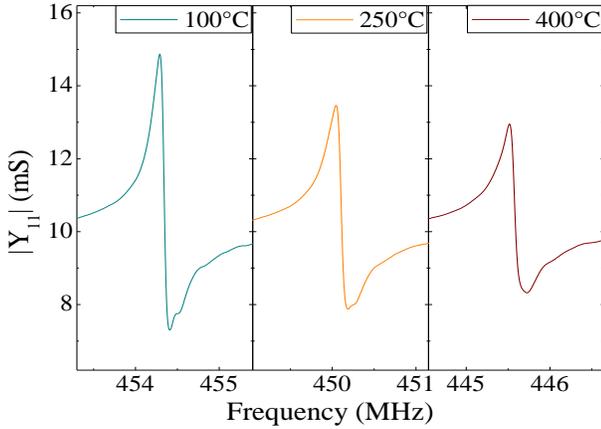


Fig. 6. Admittance spectra extracted from high-temperature characterization of optimized resonators ($\lambda_{\text{IDT}} = 12.64 \mu\text{m}$). Spectra show very clear parallel and series resonances, in spite of a moderate increase in impedance mismatch with temperature.

When heated up to 450°C, the resonators can still sustain RF measurements, but at the cost of a decrease of the signal. Contrary to previous cycles up to 400°C, the initial performance of the optimized resonators could not be recovered after cooling. It can be explained by the behavior of the Al electrodes: they require passivation for proper operation with this optimized design, which is much more sensitive to the electrical behavior of the electrodes. It then results in a progressive impedance mismatch, that explains the observed signal loss at temperatures higher than 450°C, compared to the results obtained on the standard resonator design. However, the characterization of the optimized resonators for cycles up to 400°C leads to a clean, more linear TCF behavior, with a low drift through the successive heating and cooling cycles (Figure 7). The first-order TCF is $-57 \text{ ppm}/^\circ\text{C}$, while the second-order TCF is $-17 \text{ ppb}/^\circ\text{C}^2$. This is again in good agreement with previous results, for a relative AlN thickness of 0.24 [25]. The temperature reading errors are particularly low, in spite of the limited resolution of the chuck's temperature display (1°C), that served as a reference.

A further analysis of the high temperature spectra has been performed, in order to retrieve the quality factor and the effective coupling coefficient as a function of temperature (Figure 8). The quality factor, while decreasing with temperature, remained high up to 400°C, and sustained several heating cycles up to this temperature. At 400°C, it is still at 50% of its room temperature value, which is well enough for proper wireless operation. The effective coupling coefficient follows an inverse trend, with a regular increase with temperature. Overall, the $Q \cdot k_{\text{eff}}^2$ maintains well through the whole temperature cycles, which goes along with the expectedly good preservation of the piezoelectric properties of the AlN layer at high temperatures. However, higher temperatures tend to strongly decrease the performance of the optimized resonators.

When the temperature reached 450°C, a stronger decrease of the quality factor was noticed, down to 2900.

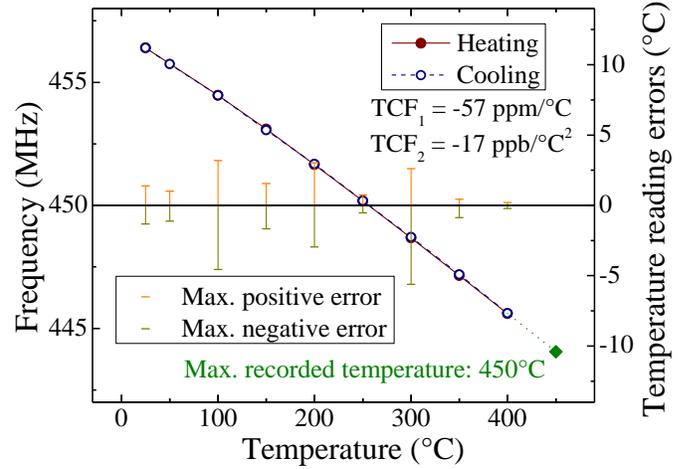


Fig. 7. TCF curve and temperature reading errors of an optimized resonator ($\lambda_{\text{IDT}} = 12.64 \mu\text{m}$), showing very good reversibility and repeatability in temperature reading up to 400°C. Signal loss happens when temperature is increased and maintained to 450°C.

A variant of these optimized resonators, with higher metallization ratio (MR = 60%), was also tested. Their quality factor was expectedly lower (4820 at room temperature), and their coupling coefficient higher (0.051%). The resulting figure of merit was similar at room temperature, and nearly constant up to 400°C (as shown in Figure 8, for comparison purposes). Their better overall stability can be explained by the lesser resistance of their larger IDT fingers, which indicates that a proper passivation of the electrodes could bring more stability at high temperature.

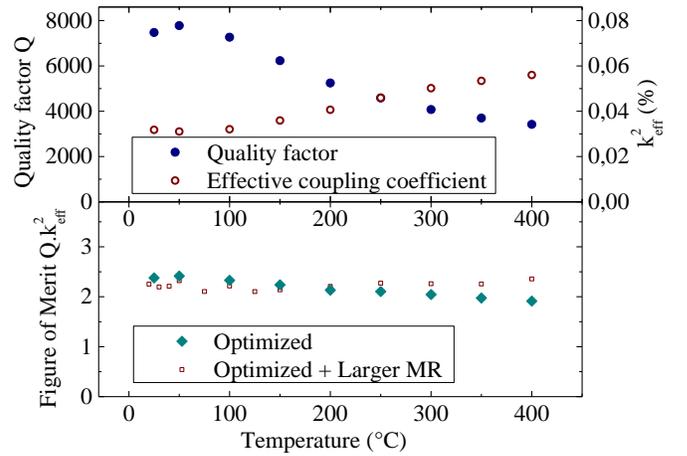


Fig. 8. Room temperature characterization of optimized quasi-synchronous SAW resonators ($\lambda_{\text{IDT}} = 12.64 \mu\text{m}$), exhibiting largely improved quality factor (8140) and cleaner S_{11} spectrum.

IV. CONCLUSION

To conclude, this paper presented the exploration of thick and high-quality aluminium nitride layers on sapphire for the fabrication of high quality factor SAW resonators in the 433 MHz ISM band. The high thermal stability of the aluminium

nitride synchronous resonators has been proven up to 600°C using standard aluminium electrodes. Based on these first measurements, quasi-synchronous optimized resonators were designed, with a Q -factor higher than 8000. This design was validated up to 400°C, with quality factors remaining as high as 3400 at this temperature, which remains large enough for the future exploitation of the resonators as wireless temperature sensors. Meanwhile, the figure of merit shows a limited loss of 20% compared to room temperature.

The perturbations occurring at 450°C are the result of the larger sensitivity of the optimized design to the electrical behavior of the electrodes which encounters steady oxidation process, leading to a detuning of the resonators. This leads to a stronger, unrecoverable loss in the quality factor and in the figure of merit. The high temperature behavior of the complete resonator structure will then have to be taken into account in the optimization process.

Overall, this paper proves that it is possible to design wireless sensors based on AlN/Sapphire SAW resonators, which now opens new challenges for compatible electrodes. A trade-off needs to be found between their acoustic properties, and their chemical stability at high temperature. Once passivated, aluminium can still be considered for this purpose, in order to reach longer lifespans and larger temperatures for sustained use of SAW sensors based on aluminium nitride.

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