AlN/ZnO/LiNbO 3 Packageless Structure as a Low-Profile Sensor for Potential On-Body Applications

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Abstract— Surface acoustic wave (SAW) sensors find their application in a growing number of fields. This interest stems in particular from their passive nature and the possibility of remote interrogation. Still, the sensor package, due to its size, remains an obstacle for some applications. In this regard, packageless solutions are very promising. This paper describes the potential of the AlN/ZnO/LiNbO$_3$ structure for packageless acoustic wave sensors. This structure, based on the waveguided acoustic wave principle, is studied numerically and experimentally. According to the COMSOL simulations, a wave, whose particle displacement is similar to a Rayleigh wave, is confined within the structure when the AlN film is thick enough. This result is confirmed by comprehensive experimental tests, thus proving the potential of this structure for packageless applications, notably temperature sensing.

***Index Terms*— Surface acoustic wave SAW, temperature sensor, waveguiding layer acoustic wave WLAW, packageless, low-profile.**

I. Introduction

This paper is an extended version of the conference paper [1] presented at the IEEE International Ultrasonics Symposium 2017 in Washington, USA.

Surface Acoustic Wave (SAW) devices are widely used in communication systems as filters or resonators [2]. Thanks to the sensitivity of the resonance frequency to some physical parameters of the environment (for example the temperature), the devices can be also used as sensors. Because SAW sensors can be remotely interrogated (wirelessly) and because they are passive (batteryless), this allows them to be used in a wide range of Radio Frequency (RF) applications [3-7] in various areas, including medicine and sports. Indeed, there is a need for monitoring the data or the parameters of the human body. A limitation to this growing trend remains the presence of the package. The package is useful to protect the device from external perturbations (such as humidity) and for the stress isolation but it is also expensive and bulky. Consequently, the package prevents close contact between the sensor and the target, i.e. the human body. To eliminate this bottleneck, some authors have suggested a bilayer structure with AlN and LiNbO$_3$ 128° Y-cut [8]. The confinement of the energy is possible due to the use of heavy metal electrodes (Pt) and occurs mostly owing to specific properties of LiNbO$_3$ 128° Y-cut which shows a decoupling between Rayleigh modes and Shear Horizontal modes. The Waveguiding Layer Acoustic Wave (WLAW) principle is another way to overcome this limitation and to develop a new generation of wireless on-skin sensors [9-11]. In this structure, the acoustic wave is confined in a low velocity film placed inbetween two high velocity materials (see Fig.1). This paper investigates the AlN/ZnO/LiNbO$_3$ (128° Y-cut) structure as a candidate for a WLAW temperature sensor. The ultimate goal is to realize several multifunction sensors and thus to use a reflective delay-line including an ID-Tag. This configuration requires the use of a piezoelectric substrate that has a large electromechanical coupling coefficient (K^2) and low propagation losses. Thus, in this work we will try to maximize the K^2 value of the entire structure. However, for practical considerations, a resonator structure will be considered in this paper. Indeed, the design and manufacturing are easier and the theoretical study can be done considering a single cell of the IDT. This makes the calculations for the structure optimization less time consuming, while enabling the investigation of the wave confinement in this structure, which is the *sine qua non* feature for packageless applications.

The LiNbO$_3$ 128° Y-cut was chosen for its high electromechanical coupling coefficient K^2 (K^2=5.4 %) and its relatively high acoustic velocity to play the role of the piezoelectric substrate used to generate the acoustic wave [12,13]. The ZnO and the AlN layers are used as a low and a fast velocity layer respectively, in order to build the packageless structure [14-16].

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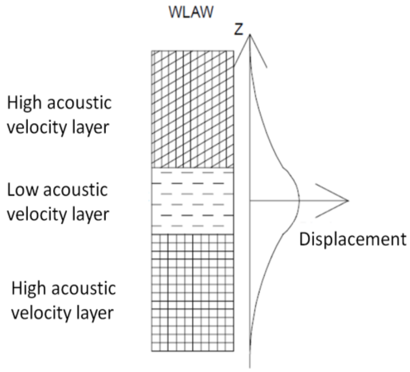

Fig. 1. Principle of the WLAW structure (adapted from [9]). One of the layers needs to be piezoelectric.

II. Materials and methods

A. FEM Modeling

The structure was studied by a 3D-FEM modeling (COMSOL Multiphysics®), using anti-periodic boundary conditions along the X-axis. Physical constants of considered materials were extracted from the literature for AlN and $LiNbO_3$ [17,18] and by using Comsol Multiphysics® library for ZnO and gold. $LiNbO_3$ is considered as a piezoelectric material to generate the SAW response. AlN and ZnO have also been considered as piezoelectric materials insofar as it has been verified that this feature generates negligible orders of magnitude compared to those due to the elastic constants of the layers. Firstly, only the structure with $LiNbO_3$ and the gold electrodes was calculated and the results were compared to experimental ones. ZnO and AlN layers were then added in the model and their thicknesses were adjusted in order to provide a good electromechanical coupling coefficient (K^2). The maximization of the K^2 value to a certain level is usually appreciable because it reflects the efficiency of conversion between the electrical and the acoustic energy in the piezoelectric material. The minimum AlN thickness required for the wave confinement was finally predicted by the simulations.

B. Experimental part

To yield sensors operating in the 868 MHz ISM band, (Ti 10nm/Au 90nm) SAW devices with a wavelength of 4.4 µm were patterned on the piezoelectric $LiNbO_3$ 128° Y-cut substrate (MTI Corporation) using e-beam lithography (see Fig.2b and 2c). This synchronous resonator has 100 finger pairs and 200 reflectors on each side. Ion beam etching (IBE) was used to etch the (Ti 10nm/Au 90nm) layers, followed by O_2-plasma treatment to remove the negative resist. Fig.2a, gives a first idea of the future wireless structure. The WLAW structure, based on the resonator configuration, in the center is attached to flexible antennas made of Kapton sheets.

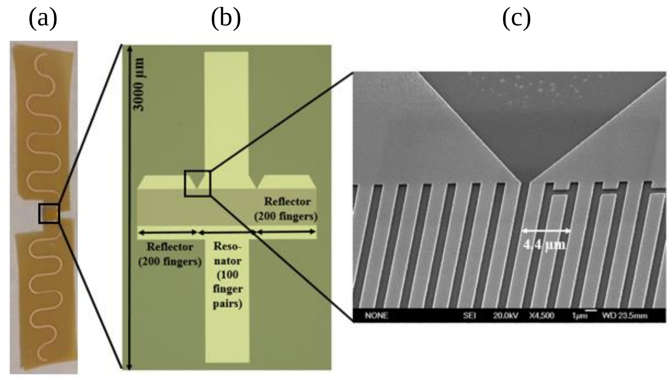

Fig. 2. Top view of finale structure, including the sensor and a flexible antenna (a), and the fabricated SAW device (b and c)

The ZnO and AlN layers were then successively deposited on the top of the electrodes using reactive magnetron sputtering with the following parameters:

TABLE I
Summary of deposition parameters

	ZnO	AlN
Target	ZnO (Ø 4-inch)	Al (Ø 4-inch)
Gases	6 sccm* O_2 6 sccm* Ar	16 sccm* N_2
Temperature	170°C	No intentional heating
Target power	150 W	200 W
Total pressure	$6x10^{-3}$ mbar	$8x10^{-3}$ mbar

**sccm: standard cubic centimeters per minute (flow unit)*

The AlN deposition was performed in several steps with intermediate measurements of the resonator frequency response in order to observe the evolution of the confinement of the wave with respect to the thickness of AlN. To keep the contact with pads for the measurements, a physical shadow masking was used during the deposition steps. SAW devices were characterized using a probe station (Suss Microtech PM5) and a network analyzer (VNA Agilent-N5230A). The probe station is equipped with a thermal chuck allowing the control of the temperature between 20 and 100°C with a precision of 0.1°C.

In order to verify experimentally the confinement of the wave in the WLAW device, we investigated the effect of addition of a soft elastomeric matter on top of it: if no change in the S-parameters is observed, then it proves that the wave is confined (see Fig.3).

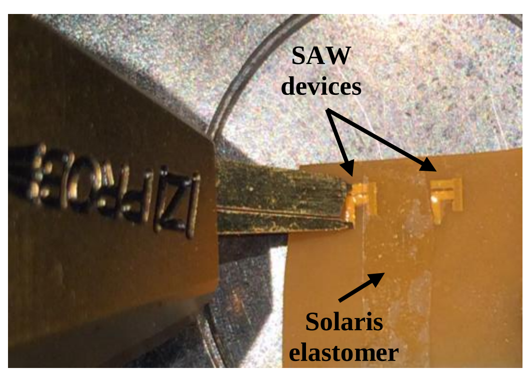

Fig. 3. Measurement of S-parameters with the silicone elastomer Solaris on top of the device after ZnO and AlN depositions.

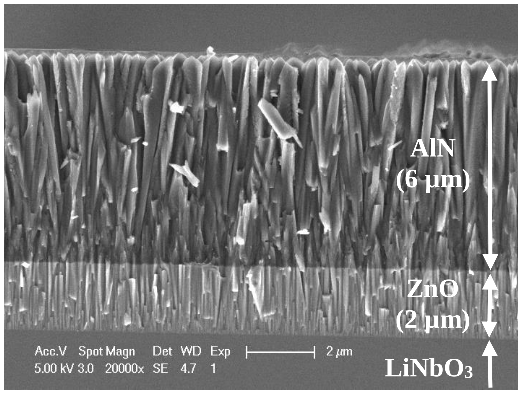

Fig. 4. SEM cross-sectional image of the AlN/ZnO/$LiNbO_3$ structure.

To remain as close as possible to the intended application, an absorber with almost the same properties as the skin such as the Solaris elastomer (Smooth-on, USA, E_{Young}=172 kPa) has been chosen. Finally, scanning electron microscopy (SEM) was used to check the thickness of the deposited films (see Fig.4).

III. Results

A. FEM Modeling

Initial calculations were performed using a top and a bottom layer with a thickness large enough to ensure the confinement of the wave on each side. In this configuration it has thus been found that 2 µm provides a good value for the ZnO layer thickness. Indeed, with this thickness, the K^2 value remains high enough (more than 4%) to achieve future reflective delay-lines while the wave propagation is mainly confined around the ZnO/$LiNbO_3$ interface. Moreover, we show that the required thickness of AlN to ensure the wave isolation is limited to several microns. The model used for the resonator description will serve as a basis for the delay-lines modeling and design, after experimental verification and parameters extraction.

The numerical criterion we used to assess the wave confinement is the following: a wave is considered confined when the surface displacement is less than 1% of the waves' maximum displacement.

With the fixed value of 2 µm of ZnO, 7.5 µm of AlN, or more, are required to fully confine all the waves between 580 and 1100 MHz. Focusing on the wave at 837 MHz, the simulations even predicts that an AlN thickness of 5 µm is sufficient to confine this particular wave. In order to maintain a security margin for the manufacturing process, the value of 6 µm has been selected.

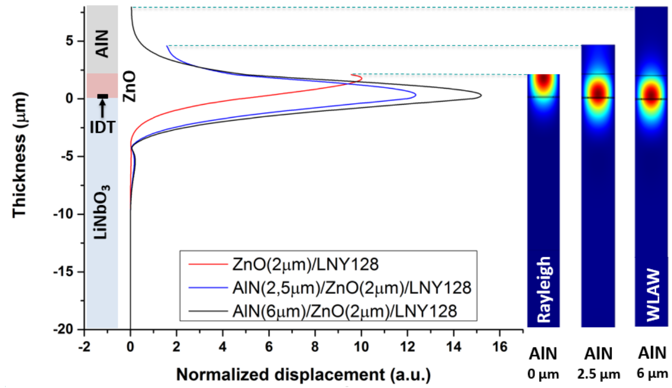

Fig. 5. Total particle displacement evolution as a function of the AlN thickness (1D display on the left, 2D on the right).

Fig.5 shows, for three different AlN thicknesses, the particle displacement along the Z-axis (normal to the surface structure) when a voltage is applied on the Inter-Digital Transducers (IDTs). Compared to the cases with 0 or 2.5 µm of AlN, the displacement at the surface of the structure is much more limited when the AlN thickness is 6 µm (less than 1% of the maximum displacement).

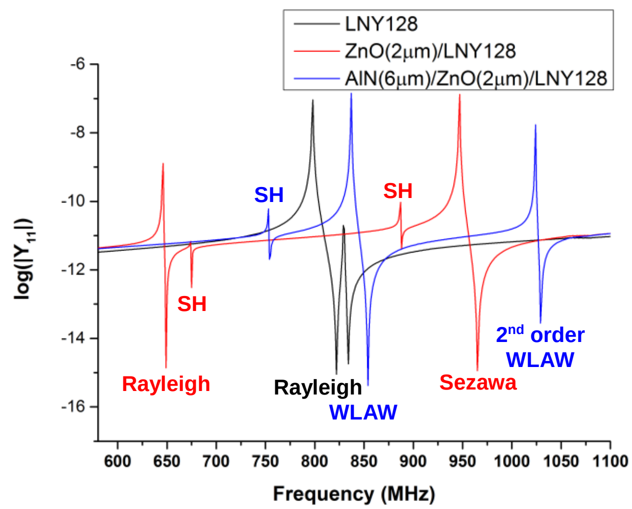

Fig. 6. Theoretical evolution of the admittance Y_{11} magnitude as a function of the frequency, for different configurations.

Fig.6 depicts the evolution of the calculated admittance magnitude for the different structures, as well as the identified modes. This figure also highlights the frequency shifts due to the presence of additional layers.

From the 3D simulations, 2D projections of the displacements in the X, Y and Z directions were created to identify those different waves (Table II). It was also possible to track the evolution of each mode when layers of different thicknesses were added to the model.

Table II shows some of those modes: Rayleigh modes are characterized by the absence of Y displacement and a large Z displacement, whereas Shear Horizontal (SH) modes display large Y displacement. For growing AlN thicknesses (6 µm), we observe a confined wave with a displacement similar to a Rayleigh wave (noted WLAW), as well as a confined SH-type wave.

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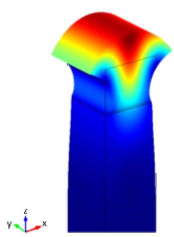
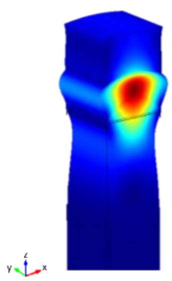
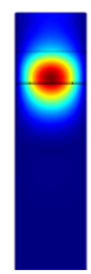
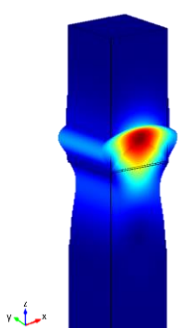
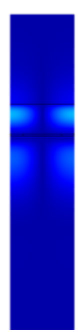
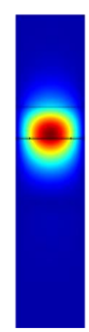
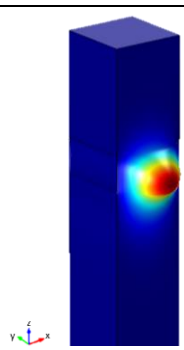
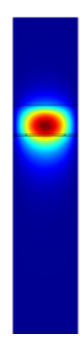
B. Impedance measurements and discussion

Impedance measurements confirm the change in frequency due to additional layers. $LiNbO_3$ is characterized as a material with a high propagation velocity with respect to ZnO [12,13]. Therefore, the $ZnO/LiNbO_3$ bilayer structure shows lower acoustic velocities than those of the substrate alone, and thus lower operating frequencies as shown by the impedance measurements (see Fig.7). The AlN layer has also a high propagation velocity [14], so according to the same principle, the average velocity of the $AlN/ZnO/LiNbO_3$ structure is higher than that of the $ZnO/LiNbO_3$ bilayer structure.

TABLE II: NUMERICAL EVALUATION OF THE PARTICLE DISPLACEMENT IN THE STRUCTURE FOR SOME RELEVANT MODES

Structure *Wave type*	Total displacement	Displacement along X-axis	Displacement along Y-axis	Displacement along Z-axis
ZnO(2µm)/LNY128 *Rayleigh wave* ***at 643 MHz***				
AlN(2.5µm)/ZnO(2µm)/LNY128 *Similar to a Rayleigh wave* ***at 835 MHz***				
AlN(6µm)/ZnO(2µm)/LNY128 *Similar to a Rayleigh wave* ***at 837 MHz*** *(WLAW)*				
AlN(6µm)/ZnO(2µm)/LNY128 *Similar to a SH wave* ***at 753 MHz***				

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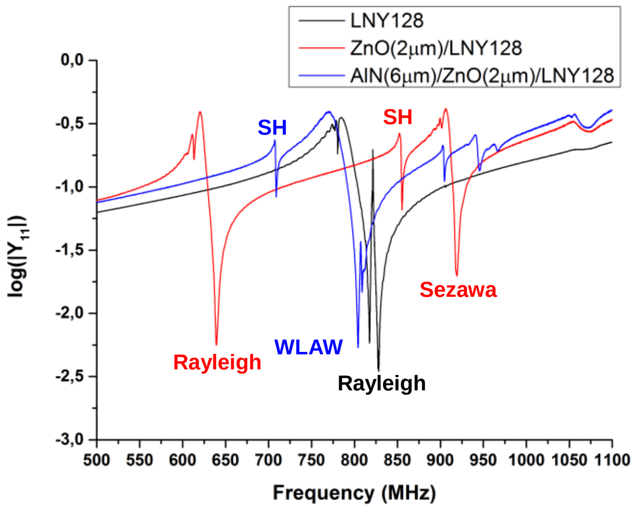

Fig. 7. Evolution of the measured admittance Y_{11} magnitude as a function of the frequency, for different configurations.

The K^2 values can be evaluated with the approximation:

$$K^2 = \frac{2(f_r - f_a)}{f_r}$$

where f_r and f_a are the resonance and anti-resonance frequencies, respectively extracted from Fig.6 or 7. In the theoretical case the estimated value is around 4%. In the experimental case, it is unfortunately difficult to determine the f_r value for the K^2 calculation. The K^2 approximation with a rough value for f_r is nevertheless promising because greater than 6%. Future achievements are needed to confirm this value and to explain the difference with the theoretical value.

Fig.8, shows the measured conductance of the resonator (G=Real(Y)) versus the frequency of the AlN/ZnO/$LiNbO_3$ structure. The experimental value of the Q factor is estimated by the inverse of fractional bandwidth between frequencies where the conductance value becomes the half of the peak [19]. The unloaded Q-factor achieved is close to 450 which is low to ensure a high sensitivity needed for a wireless sensor. This low value is in part due to the quality of the polycrystalline ZnO thin film that should be improved. Still, to allow wireless measurement, not only the Q value is important, but also the K^2. Indeed, following [20] the efficiency of energy re-radiation requires that the product $Q \cdot K_C$ be over 4, where $K_C = C_S/C$, C being the motional capacitance and C_S being the static capacitance in the resonator equivalent circuit; their ratio strongly depends on K^2.

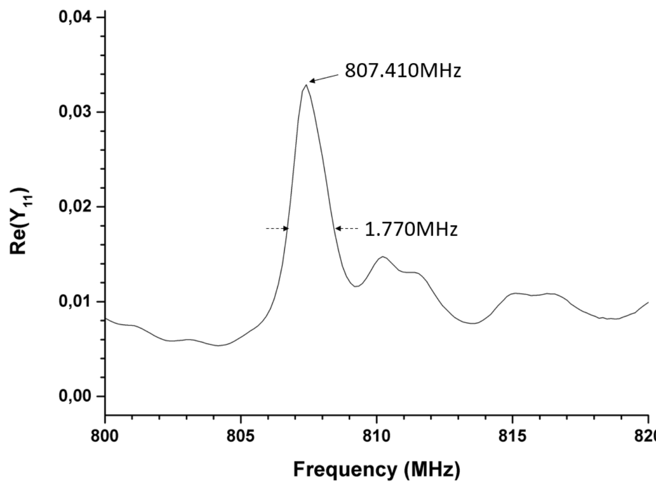

Fig. 8. Measured resonator conductance versus the frequency.

In addition, tests with the silicone-based Solaris elastomer (see II.B) were carried out to prove the wave confinement. For practical purposes, devices with longer access pads were used as shown in Fig.3. Indeed, without AlN top layer, the Solaris slab, placed on top of the structure disturbs the S_{11} signal (see Fig.9, top). On the opposite, in the structure with 6 µm of AlN, the wave at 790 MHz do not experience any change in impedance when the absorber is placed on top of it. This proves the confinement for this particular wave, noted WLAW (see Fig.9, middle). To push the analysis further, it can be noticed that the wave around 950 MHz is still disturbed by the Solaris elastomer in this configuration. This higher order mode is only confined with a thicker AlN film, e.g. with 8 µm of AlN no more changes occur (see Fig.9, bottom). In conclusion, the proposed structure is validated for packageless applications. The ZnO and AlN layers act as a package and protect the wave from external perturbations such as moisture.

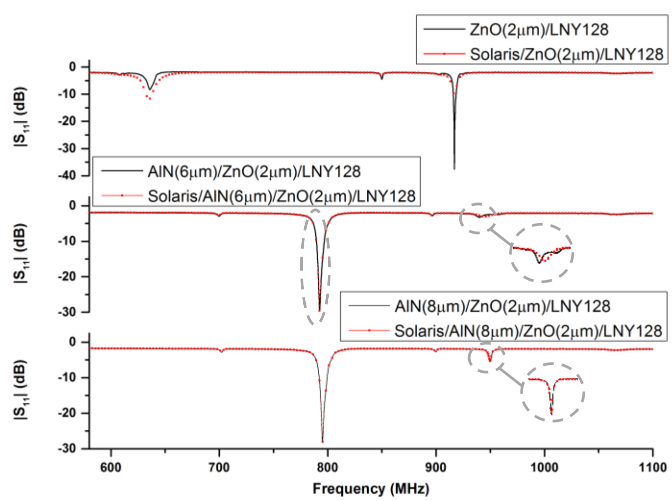

Fig. 9. Experimental evolution of the S_{11} magnitude as a function of frequency.

The structure with 6 µm of AlN, where only the WLAW wave at 790 MHz is confined, is still of interest because it could be used as a compensated sensor. On the one hand, the isolated wave is independent of the surface perturbation and can therefore be used as a reference, for example as a temperature sensor. On the other hand, the non-isolated wave is sensitive to a perturbation on the surface and can thus serve as a gas or humidity sensor while removing the temperature influence.

C. Temperature sensing potential of the structure

The temperature coefficient of frequency (TCF) of some modes was determined from the evolution of the operating frequency as a function of temperature (see Fig.10). The TCF is calculated using the equation:

$$TCF = \frac{1}{f_0}\frac{\Delta f}{\Delta T}$$

where f_0 is the operating frequency of the device at room temperature.

TCF measurements show, as expected from the literature [13], a value of -78 ppm/°C when only the substrate ($LiNbO_3$ 128° Y-cut) and the gold IDTs are measured. For the WLAW structure AlN(6µm)/ZnO(2µm)/$LiNbO_3$, a noticeably high value of -106 ppm/°C was measured. Thus, a high sensitivity is expected for temperature sensors based on the WLAW structure. Indeed, for devices operating in the 868 MHz ISM band and assuming that the electronic reader has a detection limit of 10 kHz, the sensor precision is expected to be around 0.1°C.

The frequency shift in the S_{11} curves due to the temperature increase illustrate the experimental method used (see Fig.11). From those measurements we also extracted the TCF of the first peak corresponding to SH wave around 700 MHz and to those of the higher modes recorded around 900 and 950 MHz. Their respective TCF values are: -90.8; -92.4 and -102.3 ppm/°C.

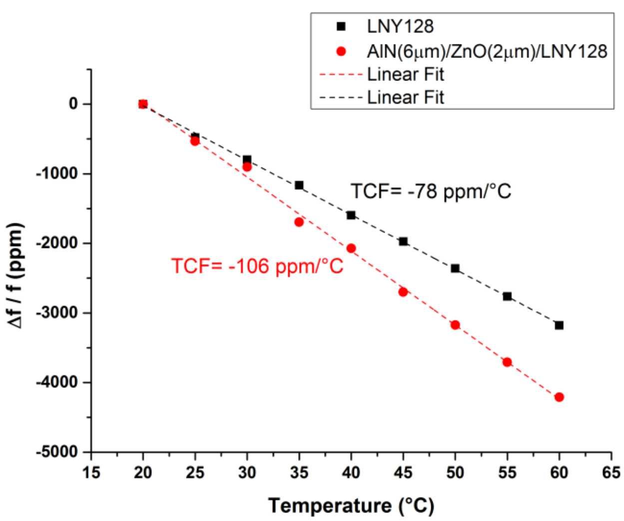

Fig. 10. Relative frequency shifts with respect to the temperature.

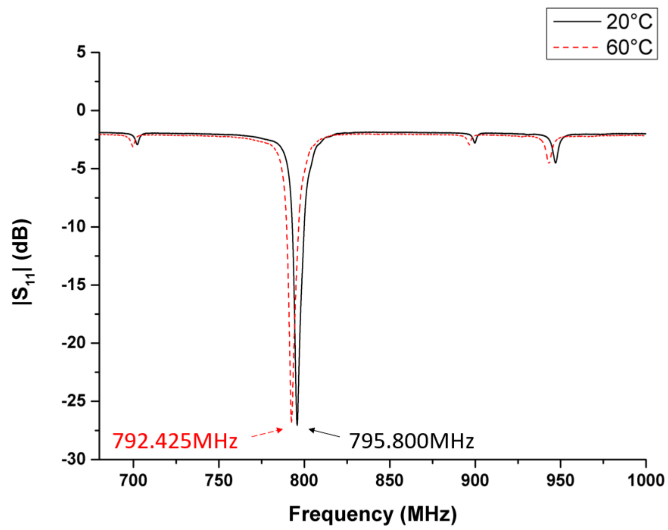

Fig. 11. Experimental S_{11} signal measurements at 20 and 60°C.

IV. Conclusion and Perspectives

The numerical and experimental measurements have allowed to obtain a better understanding of the AlN/ZnO/$LiNbO_3$ (128° Y-cut) acoustic waves structure: the different modes and the changes in velocities (and thus in the resonance frequencies) with each layer addition as a function of the relative hardnesses.

Impedance measurements, insensitive to the presence of an elastomeric absorber, led to the demonstration of the confinement of a WLAW wave, in the configuration with 2 µm of ZnO and 6 µm of AlN.

This result is in agreement with the COMSOL simulations that predicted a sufficient value of 5 µm (or 6 µm with some reasonable margin) of AlN to observe the confinement of the WLAW wave.

Hence, the AlN/ZnO/$LiNbO_3$ (128° Y-cut) structure has been validated for packageless applications. Moreover, TCF measurements show promises for on-body temperature sensing applications.

As a short term perspective, the aim is to improve the quality factor Q of the devices, which requires to reduce the acoustic losses. In the present case the wave propagation takes place mainly in the ZnO layer which has been deposited by magnetron sputtering. By forcing the wave to propagate in the single crystal lithium niobate substrate rather than in the ZnO layer, losses can be reduced. Diamond, which is harder than AlN may then be considered for the upper layer [21]. Comparison between the two structures AlN/ZnO/$LiNbO_3$ and Diamond/ZnO/$LiNbO_3$ are in progress [22]. In order to obtain low-profile sensors, the manufacturing of SAW devices on thinned substrates is also interesting.

Additionally, the manufacturing of flexible antennas will be performed in order to yield complete wireless sensors based on the WLAW structure. The final sensor will be fixed on the human body for temperature measurements, and the elastic property of the antennas will compensate the strain due to the skin deformation. For the first experiment, antennas were made with Kapton sheets with a thickness of 25 µm. Fig.2a gives an overview of the final structure where the AlN/ZnO/$LiNbO_3$ (128° Y-cut) WLAW structure is placed in the center and fixed to the antennas.

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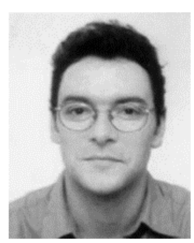

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