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ZnO/AlN Stacked BAW Resonators with Double Resonance

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Abstract— **We have fabricated BAW resonators with a piezoelectric bilayer that combines ZnO and AlN films. These stacked devices show two resonances that could be used to simultaneously track temperature variations and another parameter, such as loaded mass or pressure. We have assessed the crystal quality of the stacked piezoelectric films using XRD and FT-IR. The TCF of the devices has been measured in a temperature range from 25°C to 100°C. Both resonances show different TCFs, of -15.8 (ppm/°C) and -19.9 (ppm/°C), and quality factors Q over 500, which make them suitable for measurement of two parameters.**

Keywords—Stacked resonators, Solidly mounted resonators, AlN, ZnO, TCF

I. INTRODUCTION

During the last decade, bulk acoustic wave (BAW) resonators based on piezoelectric thin films have raised an increasing interest among the industrial and scientific community. Their applications in mobile communications, using them to fabricate multiplexers and filters, and in bio and gas sensing, thanks to their sensitivity to mass variations, are widely reported [1-3]. The operating principle of this kind of device relies on an acoustic resonance that is generated in the piezoelectric thin film, sandwiched between two conducting electrodes, by applying an electric signal.

Two different structures are commonly used to confine the acoustic energy within the piezoelectric material. The free-standing bulk acoustic wave resonators (FBARs) ensure the reflection of the wave by suspending the resonator on an air gap [4]. In the solidly mounted resonators (SMRs) the confinement of the acoustic energy is achieved by the use of an acoustic reflector (Bragg mirror), which consists of a stack of alternated layers of high acoustic impedance and low acoustic impedance materials with λ/4 thicknesses [5].

Usually, the piezoelectric material for BAW resonators is chosen to be either AlN or ZnO [6,7]. It is unusual to combine both, but some work has been done looking for an adequate seed layer that improves the growth of the piezoelectric layer. The benefits of this method have been observed in AlN seeding ZnO layers rather than in ZnO seeding AlN layers [8].

Stacking of piezoelectric materials has been investigated to fabricate coupled filters. These structures usually use two different layers of the same piezoelectric material, which are separated by some coupling layers that act as a second acoustic reflector. These structures allow the fabrication of higher order filters without an increase in the manufacturing costs [9].

Regardless of the application, resonant frequency variations due to temperature changes are one of the main concerns because they can lead to the malfunction of the device. For example, the stability in bandwidth and band frequency of a filter can be altered if the resonant frequency of the devices varies. A shift of the resonant frequency with temperature changes of a gravimetric biosensor is even more dramatic, because it could generate a false positive. One of the solutions that has been adopted, especially in the area of sensors, is the simultaneous measurement of temperature and another parameter of interest, for example pressure or, commonly, mass loading, so that both variations can be independently identified [10,11]. This technique requires the generation of another resonant peak by increasing the thickness of a SiO_2 layer located below the piezoelectric layer, which causes a decrease in the quality factor of the device. With this aim, the use of two piezoelectric materials is expected to reinforce the coupled resonances, thus allowing simultaneous good quality factors in both of them.

In this paper we propose a novel approach to the stacked resonators with a potential application in simultaneous measurement of temperature and another parameter. We have fabricated SMRs with a stacked piezoelectric layer of ZnO on AlN or AlN on ZnO without any coupling layers between them. We have characterised the structure of the stacked film and measured the TCF of both modes in test devices to verify that they can be used to independently assess temperature and another parameter such as mass loading.

II. EXPERIMENTAL

We fabricated the test SMRs on (001)-oriented silicon wafers covered with an acoustic reflector made of five alternating sputtered layers of porous SiO_2 and Mo, the thicknesses of which whose thicknesses were adjusted to achieve a center frequency of 2.5-3 GHz for the longitudinal mode. We used a 120 nm-thick evaporated Ir layer as bottom electrode and a 150 nm-thick sputtered Mo layer as top electrode. Depending on the device, the piezoelectric layers sandwiched between the electrodes were deposited in different orders (ZnO on AlN or AlN on ZnO).

AlN thin films, with thicknesses ranging from 500 nm to 1200 nm, were deposited in an ultrahigh vacuum system at a base pressure ~10^{-8} Torr. A 150 mm diameter high purity Al target was sputtered in an atmosphere of 60% N_2:Ar mixture at 1.7 mTorr of total pressure. Substrate temperature was held at 400 ºC during deposition. Prior to deposition, the surface was cleaned by ion bombardment in a plasma generated by applying RF power to the substrate in a pure Ar atmosphere. This cleaning process removes around 10 nm of the Ir bottom electrode surface and but does not generate imperfections on it allowing better nucleation of the AlN film.

The piezoelectric ZnO layer was reactively sputtered at room temperature in a high target utilisation sputtering (HiTUS) system [12], as shown in figure 1, which yields high quality and low stress films [6,13]. We used a 102 mm diameter 99.999% purity Zn target. The plasma was launched at 1000 W and a power of 800 W was applied to the target in a 10:7 Ar:O_2 environment. We deposited thicknesses ranging from 500 nm to 800 nm of ZnO at a pressure of 3.4 mTorr. The substrate was rotated during deposition to enhance thickness homogeneity. No plasma etching of the substrate was performed in this case.

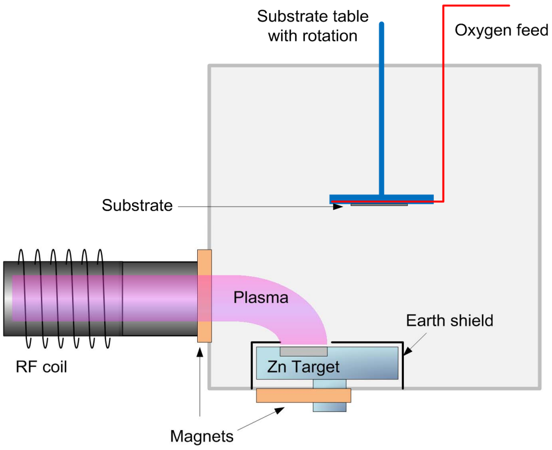

Figure 1. Schematic diagram of the HiTUS system. Thanks to its layout, the sample is always protected from the plasma, which eliminates its exposure to additional heat and ion bombardment. The substrate is rotated during deposition to achieve better uniformity of the film

The crystal structure of the piezoelectric thin film stack was assessed using reflectance infrared spectroscopy with a Perkin-Elmer Spectrum 100 extended range (7200 to 200 cm^{-1}) Fourier transform infrared (FTIR) spectrophotometer and by X-ray diffractometry measured with a Supratech XPERT-PRO diffractometer by recording the θ/2θ patterns between 30°(2θ) and 80°(2θ) using the Kα1,2 doublet of a β-filtered Cu anode. Rocking curves (RC) around the (00·2) reflections of AlN at 36.03° (2θ) and ZnO at 34.02° (2θ) were measured. After the deposition of the top electrode, we patterned the test devices and measured them with an Agilent PNA N5230A network analyzer, to study the impedance (Z) spectra between 10 MHz and 10 GHz. The spectra were fitted using a Mason model to calculate an accurate value for the effective electromechanical coupling factor (k^2_{eff}) and the quality factor at the resonant frequency (Q_r) for both resonances. We also used finite element analysis (FEA) Comsol Multiphysics software to simulate the behavior of the SMRs.

III. RESULTS AND DISCUSSION

A. *Thin film structure*

X-ray diffraction and IR spectrophotometry are commonly used to assess the crystal structure of piezoelectric thin films such as AlN or ZnO. In the case of the stacked combination of both materials, it is particularly interesting to analyze the effect on their patterns and spectra when the two piezoelectric films are measured together.

Figure 2 (a) shows the FT-IR reflection spectra of two separate layers of ZnO and AlN with their c-axis perpendicular to the surface. The different A1(LO) and A1(TO) absorbance peaks for both materials and their positions are highlighted. Below, in figure 2 (b), are the spectra of two different stacked structures, ZnO on AlN and AlN on ZnO. The AlN A1(LO) peak can be clearly identified, but the ZnO is masked by the convolution of the different absorbance peaks in the spectra (a superposition of the peaks of AlN and ZnO and also the interference fringes). A proper fit and treatment of the signal allows decomposition of the spectra and properly identification of the ZnO A1(LO) peak. The most important result obtained from these measurement is the non-appearance of the E1(LO) modes near A1(LO), indicating a pure c-axis orientation of all the analyzed layers.

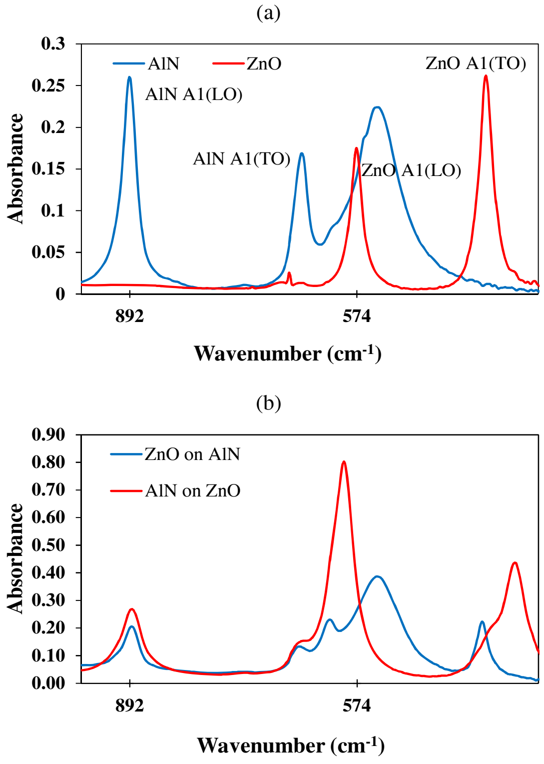

Figure 2. FT-IR spectra of AlN and ZnO individual layers (a) and stacked ZnO on AlN and AlN on ZnO structures (b). Note that the ZnO A1(LO) peak is difficult to identify in the stack, while the AlN A1(LO) is clearly visible, because of the convolution of the spectra of both materials.

This is confirmed by X-ray diffraction patterns of the stacked film, which show a similar phenomenon as the FT-IR spectra. The θ/2θ representation of individual layers of ZnO and AlN show a regular pattern, exhibiting peaks at 2θ ≈ 34° and 2θ ≈ 36º, corresponding to reflections with the <00·2> planes of the wurtzite structure of ZnO and AlN, respectively (figure 3 (a)). When the stacked structure is analyzed using XRD, a superposition of the peaks occurs and the corresponding (00·2) diffraction peaks can be identified, as observed in figure 3 (b).

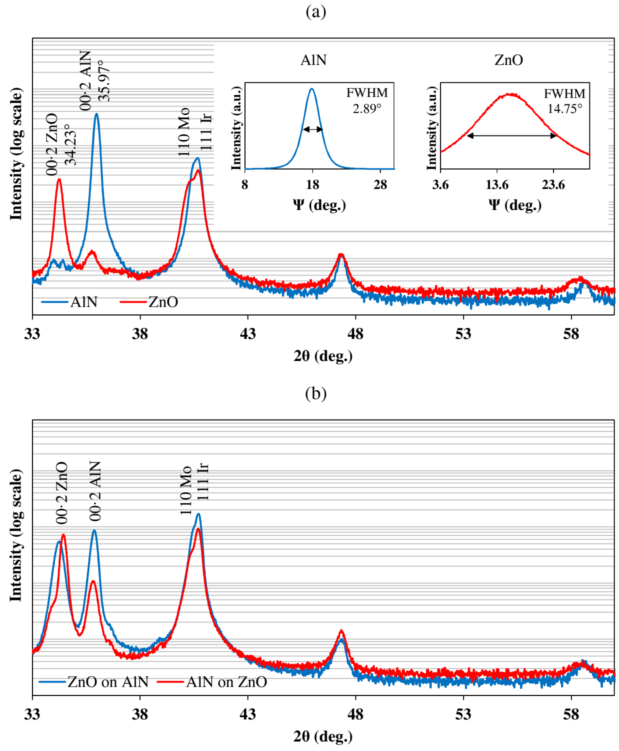

Figure 3. XRD patterns of ZnO and AlN films (a) and stacked ZnO on AlN and AlN on ZnO structures. The most relevant peaks are highlighted and the inset in (a) shows the rocking curve of both films. The poor quality of the ZnO film can be attributed to its thinness, as previously reported in [13].

XRD allows a proper assessment of the crystal quality of the piezoelectric thin films even if they are stacked, as shown in figure 4 (a) and (b). Since the (00·2) peaks appear at different diffraction angles (θ) for each material, fixing the corresponding θ value in the diffractometer allows an independent measurement of the rocking curve of each material. Note that the FWHM of the ZnO rocking curve narrows when the ZnO film is grown on top of AlN, while the rocking curve of AlN is considerably widened when the AlN film is grown on top of ZnO. The presence of oxygen on the substrate worsens the crystallographic structure of the AlN that grows on top of it and the rocking curve shows a considerably larger full-width at half maximum (FWHM).

B. Electroacoustic operation of the devices

Figure 5 shows the modulus of the impedance of two different stacked test devices, ZnO on AlN (blue) and AlN on ZnO (red). Two main resonances can be observed in both cases, which are clearly distinguishable from other spurious resonances. Their Q factors exceed 500 in all cases, which is sufficient for sensing applications. The thicknesses of the piezoelectric layers must be carefully chosen to fit the main resonances within the acoustic reflector bandwidth, allowing easy detection by the measurement of the electrical impedance of the stack.

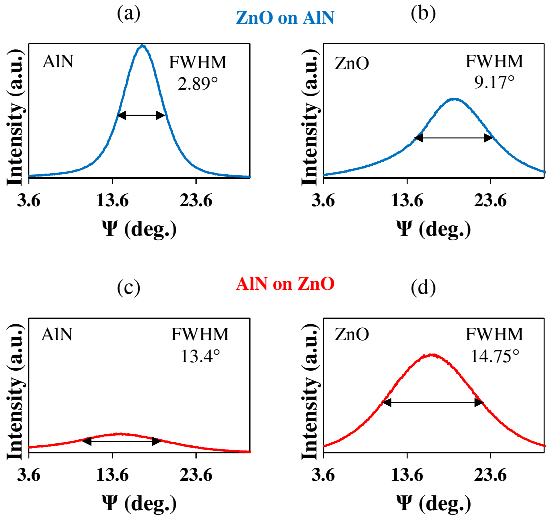

Figure 4. XRD rocking curves for a ZnO on AlN stack (a) and a AlN/ZnO stack (b). The ZnO shows a significant improvement when growing on top of AlN (increase of a 38% in its FWHM), while the AlN film quality shows a very poor structure when growing on ZnO.

There is no point in trying to get the two resonances close enough so that both of them lie within the bandwidth of the acoustic reflector. Simulations show that the loading effect produced by the piezoelectric layers in each other combined with the obvious reduction of the resonant frequency when increasing the thickness make the alignment of both modes a futile effort. To avoid acoustic energy loss at the resonant frequencies of interest, carefully designing the acoustic reflector and setting the ratio between the thicknesses of the piezoelectric materials is required. The use of free-standing structures (FBARs) for this application could improve the performance of the devices.

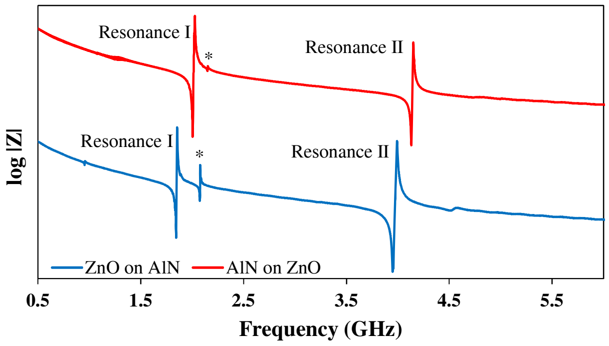

Figure 5. Electrical response of two stacked test resonators. The first one (blue) has a 700 nm AlN layer on top of 500 nm ZnO. The other (red) has a 500 nm ZnO layer on top of 800 nm AlN. The origin of the resonance marked with * is unclear. The responses have been displaced in order to improve clarity of the representation.

C. *Temperature coefficient of frequency*

One of the proposed potential applications of the stacked resonators is the simultaneous measurement of temperature and mass. To achieve this simultaneous measurement we have to ensure that both resonances vary differently as a function of temperature and mass load. Since both resonances are located at different frequencies, their response to mass load will be different, but this is not straightforward in case of their response to temperature changes.

Figure 7 shows the variation of the resonant frequency for both resonances measured in a test device of AlN on ZnO. Resonance I has a TCF of -15.8 (ppm/°C), while resonance II has a TCF of -19.9 (ppm/°C). This difference allows the use of the stacked resonators as mass sensors with temperature compensation capability.

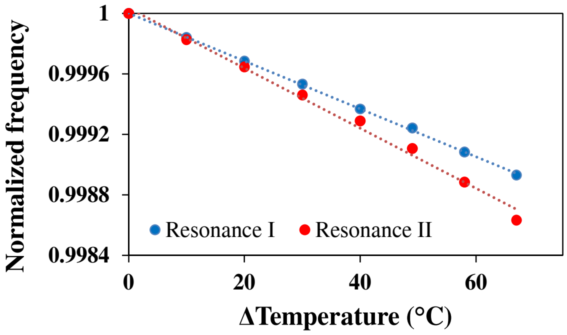

Figure 6. Variation of the resonant frequency with temperature for both resonances. Resonance I (blue) shows a TCF of -15.8 (ppm/°C) and resonance II shows a TCF of -19.9 (ppm/°C).

The values of the TCF of both resonances are surprisingly low since the single piezoelectric layer resonators have -22 ppm/ºC for AlN and -45 ppm/ºC for ZnO. The effect of the mechanical coupling reduces the TCF. Further studies of this phenomenon, also detected in the coupling of other materials [14], requires further investigation.

IV. CONCLUSIONS

We have fabricated and measured solidly mounted stacked resonators made of ZnO on AlN and AlN on ZnO films. These devices show two resonant peaks at different frequencies. We have structurally characterized the stacked piezoelectric thin films using FT-IR and XRD. Results show that XRD allows a clearer assessment of the crystal quality, because the superposition of peaks occurs at different angles. We have measured test devices and we have calculated the TCF of both resonances for an AlN on ZnO stack in a temperature range from 25°C to 100°C. The resonances I and II showed TCFs of -15.8 (ppm/°C) and -19.9 (ppm/°C) respectively, and Q over 500, which endorses the potential application of these devices as simultaneous sensors for temperature and another parameter.

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