Ta₂O₅/SiO₂ insulating acoustic mirrors for AlN-based X-band BAW resonators

GMME-CEMDATIC
E.T.S.I. de Telecomunicación.
Universidad Politécnica de Madrid
Madrid, Spain
eiborra@etsit.upm.es

V. Felmetsger
OEM Group Inc.,
Gilbert, AZ, U.S.A.

A. Devos
IEMN Dpt ISEN, UMR CNRS 8520
Lille, France
Arnaud.devos@isen.fr

Abstract— This work describes the performance of AlN-based bulk acoustic wave resonators built on top of insulating acoustic reflectors and operating at around 8 GHz. The acoustic reflectors are composed of alternate layers of amorphous Ta₂O₅ and SiO₂ deposited at room temperature by pulsed-DC reactive sputtering in Ar/O₂ atmospheres. SiO₂ layers have a porous structure that provides a low acoustic impedance of only 9.5 MRayl. Ta₂O₅ films exhibit an acoustic impedance of around 39.5 MRayl that was assessed by the picoseconds acoustic technique. These values allow to design acoustic mirrors with transmission coefficients in the centre of the band lower than -40 dB (99.998 % of reflectance) with only seven layers. The resonators were fabricated by depositing a very thin AlN film onto an iridium bottom electrode 180 nm-thick and by using Ir or Mo layers as top electrode. Resonators with effective electromechanical coupling factors of 5.7% and quality factors at the antiresonant frequency around 600 are achieved.

I. INTRODUCTION

Wireless communications systems have undergone an incredible evolution since the first mobile phones operating in 800 MHz range appeared in the market in the early 70s. Current mobile phones (GSM, WCDMA, DCS, etc.) operate at frequencies between 800 MHz and 2200 MHz. New applications, as WiMAX, extend the operation frequency to 3.5 GHz; some countries target the X-band (8 to 12 GHz) for their new mobile phone generation. Miniaturization, increasing power handling and higher transmission bands are boosting the development of more efficient circuits and components.

To obtain well-performing devices, a good acoustic isolation of the resonators is required to avoid energy losses through the substrate that reduce their quality factor. The piezoelectric stack is acoustically isolated from the substrate either by an air cavity or through an acoustic reflector, composed of a set of alternated layers of high and low acoustic impedance, in which case we obtain a solidly mounted resonator (SMR) [1]. In most cases the high acoustic impedance material used in the acoustic reflectors is a high density metal (Mo or W). If filters are the targeted application, the different metallic layers of the acoustic mirrors must be patterned to avoid crosstalk between the different resonators that form the filter. This requirement can be avoided if all the layers composing the reflector stack are insulating. Silicon dioxide (SiO₂) films are commonly used as low acoustic impedance layer, owing to their easy processing and full compatibility with standard silicon technologies [2]. Other low impedance insulating material is silicon oxycarbide (SiOC) [3], although it has the disadvantage of having elevated acoustic losses and some adherence problems. On the other hand, insulating materials with high acoustic impedance are typically aluminum nitride (AlN) [4], silicon nitride (Si₃N₄) [3] or tantalum oxide (Ta₂O₅) [5, 6]. None of these three materials really exhibits very high acoustic impedances, in comparison with that offered by high density metallic layers. The considerably large acoustic velocity of AlN combined with a low mass density provides relatively high acoustic impedance. On the other hand, Ta₂O₅ offers similar acoustic impedance than AlN by virtue of its high mass density, although its sound velocity appears to be considerably smaller.

In this work we have designed, fabricated and characterized SMRs working at around 8 GHz based on AlN capacitors built on top of all-insulating acoustic reflectors made of porous SiO₂ and amorphous Ta₂O₅. The electrical characterization of the resonators shows evidences of the better performance of Ta₂O₅-based acoustic reflectors compared to that of conventional AlN-based acoustic mirrors.

II. EXPERIMENTAL

The acoustic reflectors were composed of seven alternated layers of SiO₂ and Ta₂O₅ deposited over on silicon substrates. SiO₂ and Ta₂O₅ films were deposited in a Leybold Z-550 system by pulsed-DC magnetron sputtering of 150 nm-wide Si and Ta targets in Ar/O₂ admixtures. A pulsed-DC power of 50 kHz and duty cycle 75% was applied to the target. To tune the acoustic properties of the Ta₂O₅ films the pulsed-DC power was varied between 500 W and 1200 W, the total pressure in the chamber 1.5 mTorr and 3.3 mTorr and the percentage of O₂ in the gas between 30% and 100%. The substrates were not intentionally heated during deposition.
To achieve reproducible material properties, prior to the film deposition, the metallic target (Si or Ta) was stabilized in a pure O₂ atmosphere at constant power. The stabilization was monitored by measuring the magnetron discharge voltage as a function of time until a constant value was reached. The selected gas Ar/O₂ mixture was then fed into the chamber at the chosen pressure; the discharge voltage was again controlled until the new steady state (constant discharge voltage) was attained. At that moment the shutter was opened for film deposition during the desired time. Subsequent depositions under identical conditions required only a few minutes for stabilization. The uppermost SiO₂ layer of the reflector was mechanically polished to reduce roughness to less than 1 nm before building the AlN resonator.

The SMRs were completed by building Ir/AlN/Ir stacks on top of the acoustic reflector. Ti/Mo seed layers were used to promote the growth of highly (111)-oriented Ir layers with narrow RC (FWHM in the range of 2.5°). Ir bottom electrodes were deposited by pulsed DC sputtering at 350°C. AlN films were deposited in an Endeavor-AT PVD cluster tool of OEMGroup Inc. One of the process modules is equipped with S-Gun magnetron for alternating current (AC) (40 kHz) reactive sputtering with capability for independent control of the film crystal orientation, stress, and uniformity. The deposition rate was 48 nm/min in all experiments. Prior to AlN deposition, the substrate surface was treated by low energy Ar ions either in a separate planarized RF (13.56 MHz) etch module (PRF), producing a capacitively coupled plasma, or in the deposition module (in-situ etch). Deposition processes were performed either without external heating (T<300°C) or at elevated temperatures (up to 400°C) using an external IR heater to warm the wafer before or during deposition.

The sputtered porous SiO₂ films used as low impedance layer had been already characterized in a earlier work [7]. They were deposited in the previously set conditions that provide SiO₂ films with the lowest values of mass density (1.8 g/cm³) and acoustic longitudinal velocity (5300 m/s). The combination of these two values yields an acoustic impedance of 9.5 MΩµl.

The structure and morphology of the Ta₂O₅ films were assessed by infrared (IR) transmission and X-ray diffraction (XRD) measurements. IR transmission was measured with a Fourier transform infrared (FTIR) Nicolet 5-PC spectrophotometer, which provided the chemical bonding configuration of the films. We used non-polarized light at normal incidence over the 400 cm⁻¹ range with a spectral resolution of 4 cm⁻¹. The absorption bands corresponding to the Si substrate were eliminated by subtracting the absorbance spectrum measured in bare Si. X-ray diffraction patterns were measured in conventional Bragg-Brentano geometry in a Supratech X-Pert MRD diffractometer between 2θ = 10° and 2θ = 80°.

The assessment of the acoustic impedance of Ta₂O₅ films requires very precise measurements of their mass density, acoustic velocity, and thickness. The thickness of the Ta₂O₅ films and that of the other films involved in test devices were measured with a Veeco Dektak 150 profilometer. The density of the Ta₂O₅ layers was assessed by X-ray reflectometry (XRR) measurements using the same diffractometer operated at grazing incidence between 0.05° and 2.5°. Finally, the longitudinal sound velocity was assessed using the picosecond ultrasonic technique on test structures consisting in a SiO₂/Mo bilayer under the Ta₂O₅ film under study [8].

III. RESULTS AND DISCUSSION

A. Films characteristics

The IR transmission spectra of the Ta₂O₅ layers show two wide bands at 950 cm⁻¹ and 650 cm⁻¹, which have been associated to the Ta-O-Ta stretching mode and the O=Ta bond, respectively, of amorphous Ta₂O₅ films [9]. The spectrum of the films, (shown in Fig. 1(a)) suggest that our Ta₂O₅ layers are amorphous. X-ray diffraction measurements confirm this behavior. Fig. 1(b) shows the XRD patterns of a thin Ta₂O₅ film 200 nm thick together a 1000 nm thick film with some Ta₂O₅ nanocrystals for comparison. Additional peaks corresponding to AlN and Mo are also observed, as the films are characterized after depositing the piezoelectric stack for piezoelectric characterization.

![Figure 1](attachment://figure1.png)

Figure 1. (a) IR transmittance of a Ta₂O₅ film 200 nm thick deposited on Si. (b) XRD patterns of AlN/Ir/Ta₂O₅ stack with Ta₂O₅ film thickness of 200 nm (bottom) and 1000 nm (top).

The mass density (ρ) of the Ta₂O₅ films was derived from XRR measurement, which provides a direct assessment of ρ independently of the thickness. X-rays impinging on smooth Ta₂O₅ surfaces at grazing incidence below a critical angle (θc) are totally reflected. When the incident angle exceeds θc, the X-rays penetrate into the film and the intensity of the reflected beam drops sharply. According to [10], the density can be obtained through the measured θc. The experimental data were fitted using the commercial software RCREFSimW from IHP [11] which provided an accurate value of ρ. The values
obtained lied between 8100 kg/m$^3$ and 7800 kg/m$^3$, which are lower than the nominal mass density of Ta$_2$O$_5$ (8200 kg/m$^3$). These low values of $\rho$ could be associated either to a lack of stoichiometry (films containing oxygen in excess) or more likely to a non-packed structure associated to the amorphous structure of most of the films. The high value of the refractive index (2.26) measured at a wavelength of 400 nm confirms this hypothesis.

To assess the sound velocity we have measured the time-of-flight ($\tau$) of a longitudinal acoustic wave within the Ta$_2$O$_5$ films deposited on a SiO$_2$/Mo bilayer of known thicknesses. If the thickness $d$ of the film is known, the sound velocity is obtained by dividing $d$ by $\tau$. In this experiment, the acoustic wave is generated by means of a pump laser pulse that impinges the surface of the sample; a strong absorption takes place when the laser pulse reaches the Mo metallic layer. This radiation absorption produces a local heating and hence a strain pulse that propagates towards the surface at the longitudinal acoustic velocity. The arrival of the acoustic pulse to the surface is detected by using a second laser beam that travels through two transparent media (Ta$_2$O$_5$ and SiO$_2$ films) until it reaches the surface of the absorbing Mo layer where the longitudinal strain wave is generated. The acoustic pulse emitted from the buried Mo layer propagates towards the free surface through the transparent SiO$_2$ and Ta$_2$O$_5$ bi-layer. The arrival of the pulse at the surface is detected as a “reflectivity step” which is due to the acoustic reflection at the free surface. Such a structure is easily detected in transparent/absorbing layer. A more detailed explanation can be found in [13].

The time delay $\tau_{\text{exp}}$ deduced in our measurements includes the time-of-flight of the echo through both the SiO$_2$ layer ($\tau_{\text{SiO}_2}$) the Ta$_2$O$_5$ layer ($\tau_{\text{Ta}_2\text{O}_5}$) and hence can be written as:

$$\tau_{\text{exp}} = \tau_{\text{Ta}_2\text{O}_5} + \tau_{\text{SiO}_2} = \frac{d_{\text{Ta}_2\text{O}_5}}{v_{\text{Ta}_2\text{O}_5}} + \tau_{\text{SiO}_2}$$

Figure 2. Time of flight for several samples with different Ta$_2$O$_5$ thickness.

In order to deduce the sound velocity in the Ta$_2$O$_5$ slab ($v_{\text{Ta}_2\text{O}_5}$), we have studied the time delay at which the reflectivity step is observed for a set of Ta$_2$O$_5$ layers of different thicknesses ($d_{\text{Ta}_2\text{O}_5}$) deposited on identical acoustic reflectors. As the SiO$_2$ layer is identical for each sample, by plotting the evolution of the time-delay as a function of the Ta$_2$O$_5$ thickness and fitting the data using a linear regression (see Figure 2) we obtain the value of $v_{\text{Ta}_2\text{O}_5}$ (inverse of the slope) in that of $\tau_{\text{SiO}_2}$ (ordinate at the origin). The mean value of the sound velocity obtained by this technique is 4900 m/s$^3$.

Finally, the AlN thin films used for the resonator fabrication have been characterized by XRD by measuring the 0/20 diffraction patterns and the rocking (RC) curve around the 00.2 direction. The thickness of the AlN films varied 170 and 200 nm. All the films were highly c-axis oriented and the full width at half maximum (FWHM) of their RC ranged between 1.8° and 3°, depending on the crystal quality of the iridium bottom electrode. A complete study of the deposition process of AlN films with these very low thickesses can be found in [14].

B. Acoustic reflector simulations and SMRs assessment

In order to investigate whether these Ta$_2$O$_5$ films may contribute to optimize the performance of non-insulating acoustic reflectors, we have simulated the acoustic transmittance of mirrors composed of nine alternated layers of porous SiO$_2$ and Ta$_2$O$_5$ films and compared it with that of conventional AlN-based mirrors and that of porous SiO$_2$/Ir mirrors, whose response have been previously studied [15]. The simulations, shown in Fig. 3, suggest that Ta$_2$O$_5$-based mirrors exhibit lower transmission coefficients in a wider frequency band those based on AlN. Although the acoustic impedances of AlN and Ta$_2$O$_5$ are very similar, this behaviour is due to the better matching between the acoustic velocities of SiO$_2$ (5350 m/s$^3$) and Ta$_2$O$_5$ (4900 m/s$^3$) than those of SiO$_2$ and AlN (11000 m/s$^3$). Additionally, the dispersion of the values of the mass density and acoustic velocity does not affect significantly the performance of the reflectors in the middle of the band.

Figure 3. Simulated transmission coefficient of acoustic reflectors composed of a) porous SiO$_2$/AlN with seven layers (doted line), b) porous SiO$_2$/Ta$_2$O$_5$ with seven layers (dashed line), and c) porous SiO$_2$/Ir with five layers (solid line).

The resonant frequency is 8190 MHz. The effective coupling factor $k_{\text{eff}}^2$ calculated by the standard IEEE method for
thickness modes [16] is 5.7 % and the quality factor at the resonant and antiresonant frequencies, derived from the slope of the variation of the impedance phase with the frequency at these frequencies are $Q_r = 140$ and $Q_a = 600$, respectively. The low value of the quality factor at the resonant frequency is due to the high series resistance of the low-thickness electrodes required to achieve high resonant frequencies. This does not affect the antiresonant frequency since the current at this frequency is very low. These values are comparable with those obtained in similar resonators made on acoustic mirrors containing Ir as high impedance material, which show similar values of $k^2_{\text{eff}}$ but values of $Q_a$ of 900 [17].

In this paper we studied the performance of SiO$_2$/Ta$_2$O$_5$-based acoustic reflectors by assessing the frequency response of SMRs operating at around 8 GHz. All reflector layers were deposited by pulsed DC reactive sputtering. We have derived the acoustic properties of Ta$_2$O$_5$ films by deriving the sound velocity from picosecond acoustic measurements and the mass density from XRD. The typical sound speed in films with thickness below 300 nm is around 4000 m/s and the mass density is around 8000 kg/m$^3$, slightly lower than nominal density of Ta$_2$O$_5$. The typical acoustic impedance of Ta$_2$O$_5$ films is 39.5 MRayl, which is slightly greater than that of AIN. Resonators with effective coupling factor around 5.7 % and $Q_a$ of 600 have been obtained. Combined with a low acoustic impedance material, such as porous SiO$_2$, Ta$_2$O$_5$ films allow fabricating all-dielectric acoustic reflectors with good performances for band-X (around 8 GHz) filtering applications.

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IV. CONCLUSIONS

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