Ta_2O_5/SiO_2 insulating acoustic mirrors for AlN-based X-band BAW resonators

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***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 Ta_2O_5 and SiO_2 deposited at room temperature by pulsed-DC reactive sputtering in Ar/O2 atmospheres. SiO_2 layers have a porous structure that provides a low acoustic impedance of only 9.5 MRayl. Ta_2O_5 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 booting 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 (SiO_2) 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 oxicarbide (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 (Si_3N_4) [3] or tantalum oxide (Ta_2O_5) [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, Ta_2O_5 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 SiO_2 and amorphous Ta_2O_5. The electrical characterization of the resonators shows evidences of the better performance of Ta_2O_5-based acoustic reflectors compared to that of conventional AlN-based acoustic mirrors.

II. Experimental

The acoustic reflectors were composed of seven alternated layers of SiO_2 and Ta_2O_5 deposited over on silicon substrates. SiO_2 and Ta_2O_5 films were deposited in a Leybold Z-550 system by pulsed-DC magnetron sputtering of 150 mm-wide Si and Ta targets in Ar/O_2 admixtures. A pulsed-DC power of 50 kHz and duty cycle 75% was applied to the target. To tune the acoustic properties of the Ta_2O_5 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 O_2 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 O_2 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/O_2 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 SiO_2 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 SiO_2 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 SiO_2 films with the lowest values of mass density (1.8 g/cm^3) and acoustic longitudinal velocity (5300 m/s). The combination of these two values yields an acoustic impedance of 9.5 MRayl.

The structure and morphology of the Ta_2O_5 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} to 4000 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 XPert MRD diffractometer between $2\theta = 10°$ and $2\theta = 80°$.

The assessment of the acoustic impedance of Ta_2O_5 films requires very precise measurements of their mass density, acoustic velocity and thickness. The thickness of the Ta_2O_5 films and that of the other films involved in test devices were measured with a Veeco Dektak 150 profilometer. The density of the Ta_2O_5 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 SiO_2/Mo bilayer under the Ta_2O_5 film under study [8].

III. Results and Discussion

A. Films characteristics

The IR transmission spectra of the Ta_2O_5 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 Ta_2O_5 films [9]. The spectrum of the films, (shown in Fig. 1(a)) suggest that our Ta_2O_5 layers are amorphous. X-ray diffraction measurements confirm this behavior. Fig. 1(b) shows the XRD patterns of a thin Ta_2O_5 film 200 nm thick together a 1000 nm thick film with some Ta_2O_5 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.

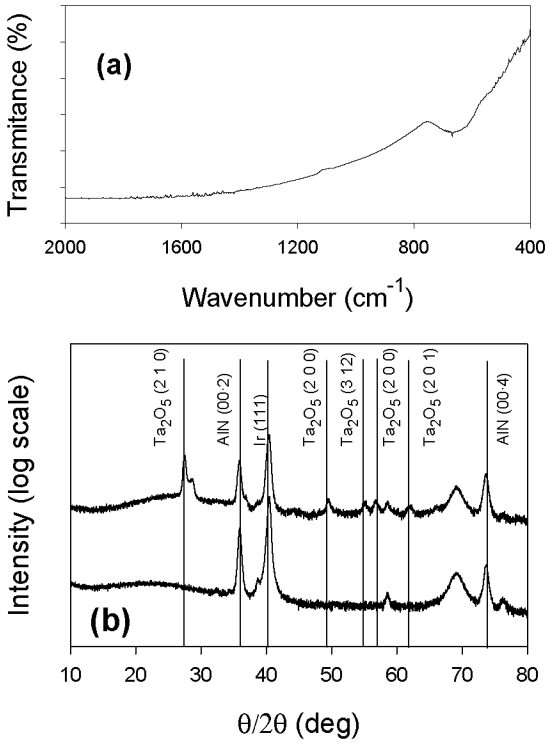

Figure 1. (a) IR transmitance of s Ta_2O_5 film 200 nm thick deposited on Si. (b) XRD patterns of AlN/Ir/Ta_2O_5 stack with Ta_2O_5 film thickness of 200 nm (bottom) and 1000 nm (top).

The mass density (ρ) of the Ta_2O_5 films was derived from XRR measurement, which provides a direct assessment of ρ independently of the thickness. X-rays impinging on smooth Ta_2O_5 surfaces at grazing incidence below a critical angle (θ_c) are totally reflected. When the incident angle exceeds θ_c, 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 θ_c. 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_2O_5 (8200 kg/m3). These low values of ρ 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 (τ) of a longitudinal acoustic wave within the Ta_2O_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 τ. 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 detect variations of the refractive index, which allows measuring the time-of-flight of the acoustic pulse in the layer under study [12]. In our samples the laser pulse travels through two transparent media (Ta_2O_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_2O_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 τ_{exp} deduced in our measurements includes the time-of-flight of the echo through both the SiO_2 layer (τ_{SiO2}) the Ta_2O_5 layer (τ_{Ta2O5}) and hence can be written as:

$$\tau_{exp} = \tau_{Ta_2O_5} + \tau_{SiO_2} = \frac{d_{Ta_2O_5}}{v_{Ta_2O_5}} + \tau_{SiO_2}$$

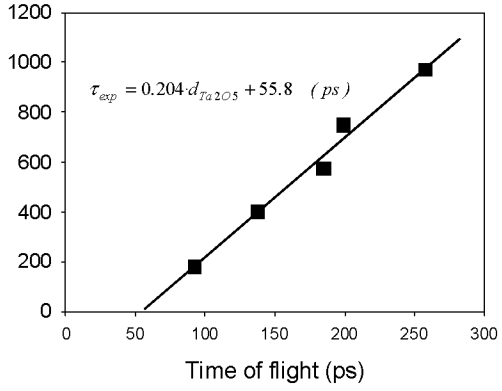

Figure 2. Time of flight for several samples with different Ta_2O_5 thickness.

In order to deduce the sound velocity in the Ta_2O_5 slab (v_{Ta2O5}), we have studied the time delay at which the reflectivity step is observed for a set of Ta_2O_5 layers of different thicknesses (d_{Ta2O5}) 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_2O_5 thickness and fitting the data using a linear regression (see Figure 2) we obtain the value of v_{Ta2O5} (inverse of the slope) in that of τ_{SiO2} (ordinate at the origin). The mean value of the sound velocity obtained by this technique is 4900 m·s^{-1}.

Finally, the AlN thin films used for the resonator fabrication have been characterized by XRD by measuring the θ/2θ 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 thicknesses can be found in [14].

B. Acosutic reflector simulations and SMRs assesment

In order to investigate whether these Ta_2O_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_2O_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_2O_5-based mirrors exhibit lower transmission coefficients in a wider frequency band those based on AlN. Although the acoustic impedances of AlN and Ta_2O_5 are very similar, this behaviour is due to the better matching between the acoustic velocities of SiO_2 (5350 ms^{-1}) and Ta_2O_5 (4900 ms^{-1}) than those of SiO_2 and AlN (11000 ms^{-1}). 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.

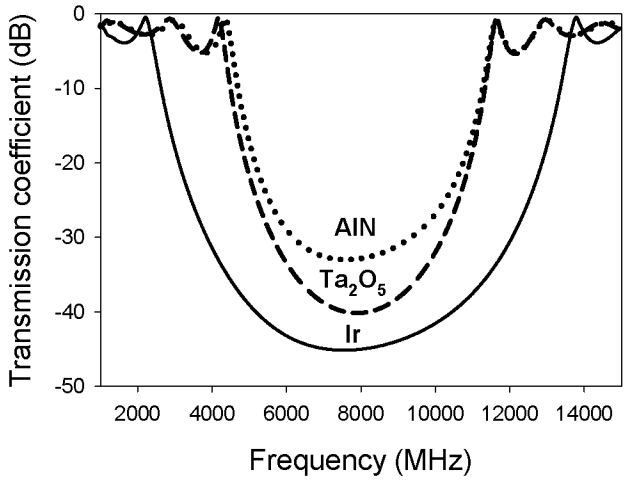

Figure 3. Simulated transmision coefficient of acoustic reflectors composed of a) porous SiO_2/AlN with seven layers (doted line), b) porous SiO_2/Ta_2O_5 with seven layers (dashed line), and c) porous SiO_2/Ir with five layers (solid line).

The response of a typical SMR is depicted in figure 4. The resonant frequency is 8190 MHz. The effective coupling factor k^2_{eff} 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_{eff} but values of Q_a of 900 [17].

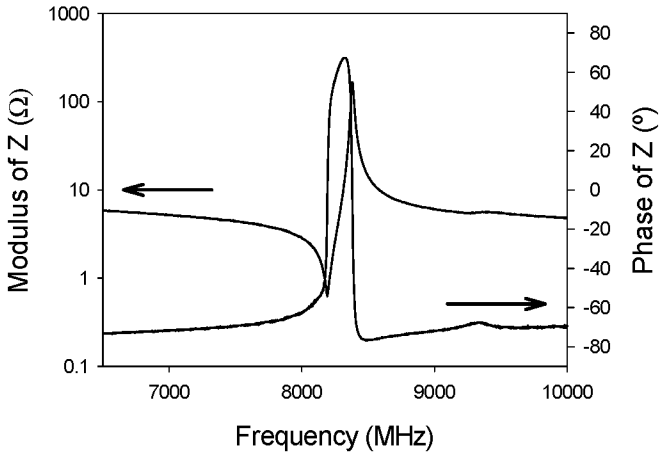

Figure 4. Impedance (modulus and phase) of a typical AlN resoantor fabricated on iinsulating acoustic reflectors made of seven porous-SiO_2 and Ta_2O_5 alternated films.

IV. Conclusions

In this paper we studied the performance of SiO_2/Ta_2O_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_2O_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 4900 m/s and the mass density is around 8000 kg/m^3, slightly lower than nominal density of Ta_2O_5. The typical acoustic impedance of Ta_2O_5 films is 39.5 MRayl, which is slightly greater than that of AlN. 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_2O_5 films allow fabricating all-dielectric acoustic reflectors with good performances for band-X (around 8 GHz) filtering applications.

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References

[1] R. Ruby, "Review and Comparison of Bulk Acoustic Wave FBAR, SMR Technology", in *Proc. 2007 IEEE International Ultrasonics Symposium*, New York 2007, 1029-10407.

[2] S. Marksteiner, J. Kaitila, G.G. Fattinger, and R. Aigner, "Optimization of Acoustic Mirrors for Solidly Mounted BAW Resonators", *in Proc. 2005 IEEE International Ultrasonics Symposium*, Rotterdam 2005, vol. 1, pp 329-332.

[3] A. Reinhardt, N. Buffet, A.Shirakawa, J. B. David, G. Parat, M. Aid, S. Joblot, P. Ancey, "Simulation of BAW resonators frequency adjustment", in *Proc. 2007 IEEE International Ultrasonics Symposium*, New York 2007, pp. 1444-1447.

[4] S.H. Kim, J.H. Kim, J.K. Lee, S.H. Lee, K. H. Yoon, "Bragg reflector thin film resonator using aluminium nitride deposited by rf sputtering", in *Proc. 2000 IEEE Microwave Conference Asia-Pacific*, Sidney 2000, pp. 1535–1538.

[5] J-W. Lobeek, R. Strijbos, A. Jansman, N. X. Li, A. B. Smolders, and N. Puisford "High-Q BAW Resonator on $Pt/Ta_2O_5/SiO_2$-based Reflector Stack", in Proc. 2007 *IEEE International MTT-S Digest*, Hawaii 2007, pp. 2047- 2050.

[6] H.P.Loebl, C.Metzmacher, R.F.Milsom, R.Mauczok, W.Brand , P.Lok, A.Tuinhout, F. Vanhelmont, "Narrow Band Bulk Acoustic Wave Filters", in *Proc. 2004 IEEE International Ultrasonics Symposium*, Montréal 2004, pp. 411-415.

[7] J. Olivares, E. Wegmann, J. Capilla, E. Iborra, M. Clement, L. Vergara, and R. Aigner, "Sputtered SiO_2 as Low Acoustic Impedance Material for Bragg Mirror Fabrication in BAW Resonators", *IEEE Trans. Ultrason. Ferr. Freq. Control.*, vol. 57 nº 1, January 2010, pp. 23-29.

[8] P. Emery, G. Caruyer, R. Vélard, N. Casanova, P. Ancey, and A. Devos, "Picosecond Ultrasonics: An original tool for physical characterization of Bragg reflectors in bulk acoustic wave resonators" in *Proc. 2005 IEEE International Ultrasonics Symposium*, Rotterdam 2005, pp. 906-909.

[9] A.P. Huang, S.L. Xu, M.K. Zhu, B. Wang, H. Yan, "Crystallization control of sputtered Ta_2O_5 thin films by substrate bias", *Appl. Phys. Lett.* vol 83, nº 16, pp. 3278-3280 (2003).

[10] A. C. Ferrari, A. Libassi, B. K. Tanner, V. Stolojan, J. Yuan, L. M. Brown, S. E. Rodil, B. Kleinsorge, J. Robertson "Density, sp3 fraction, and cross-sectional structure of amorphous carbon films determined by x-ray reflectivity and electron energy-loss spectroscopy", *Phys. Rev. B 62*, pp. 11089-11103 (2000).

[11] P. Zaumseil, Reflectivity software RCRefSimW, Version 1.09 Innovations for high performance Microelectronics. Frankfurt Germany. (http://www.ihp-microelectronics.com) (2009)

[12] P. Emery, A. Devos, P Ancey "Picosecond Ultrasonics: the preferred tool for BAW characterization" *Proc. 2008 IEEE International Ultrasonics Symposium*, Beijin 2008, pp. 2205-2208.

[13] A. Devos and R. Côte, "Strong oscillations detected by picosecond ultrasonics in silicon: Evidence for an electronic-structure effect", *Phys. Rev. B 70*, 125208 (2004).

[14] E. Iborra, M. Clement, J. Capilla, J. Olivares, V. Feltmesger, "Low-thickness high-quality aluminum nitride films for super high frequency solidly monted resonators", submitted to Thin Solid Films.

[15] J. Olivares, E. Wegmann, M. Clement, J. Capilla, E. Iborra, and J. Sangrador, "Assessment of solidly mounted resonators with wide-band asymmetric acoustic reflectors", *Proc. 2010 IEEE International Ultrasonics Symposium*, San Diego, 2010, pp. 1677-1680.

[16] IEEE Standard on piezoelctricity. ANSI/IEEE Std 176-1987.

[17] E. Iborra, M. Clement, J. Capilla, J. Olivares, and V. Felmetsger, "Optimization of thin AlN sputtered films for X-band BAW resonators", Proc. 2010 IEEE International Ultrasonics Symposium, San Diego, 2010, pp. 1688-1691.