Optimization of thin AlN sputtered films for X-band BAW resonators

E. Iborra, M. Clement, J. Capilla, J. Olivares
Grupo de Microsistemas y Materiales Electrónicos,
Universidad Politécnica de Madrid
Madrid, Spain
enrique.iborra@upm.es

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

***Abstract*—We investigate the sputter growth of very thin aluminum nitride (AlN) films on iridium electrodes for high frequency filtering applications. The structure and piezoelectric activity of AlN films are assessed through XRD, FTIR, stress and frequency response measurements. A combination of pre-deposition rf plasma treatment of the Ir bottom electrode followed by a two-step ac reactive sputtering of the AlN film allows to optimize the crystal quality and residual stress of AlN films with a thickness as low as 160 nm. BAW resonators tuned around 8 GHz are built on top of polished Bragg reflectors composed of porous SiO_2 and Ir layers. Material coupling factors k_{mat}^2 of 6.7% and quality factors Q close to 900 are achieved. The films obtained are competitive for X-band filter fabrication.**

Keywords- AlN, sputtering, high frequency BAW resonator

I. INTRODUCTION

Wireless communications systems have suffered 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. Compared to ceramic filters or SAW-based devices, BAW-based filters are the most suitable devices to meet the previous requirements offering, moreover, compatibility with ICs technologies.

BAW filters are composed by two families of BAW resonators connected trough different topologies. Such resonators consist of piezoelectric film sandwiched between two electrodes (piezoelectric stack). Aluminum nitride (AlN) is the preferred piezoelectric layer owing to its good acoustic properties and good compatibility with silicon or silicon-germanium technologies. 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).

SMRs with large effective electromechanical coupling factors (k_{eff}^2) and quality factors (Q) can be achieved by improving the piezoelectric activity of the AlN layers and optimizing the design of the reflector and the piezoelectric stack. The resonant frequency f_r is ideally set by fixing the thickness of the piezoelectric layer to $\lambda/2$; a well-designed reflector should provide the maximum isolation at this frequency. Unfortunately, in the practice, the piezoelectric stack and the reflector cannot be designed independently, as the resonant frequency and the transmission of the mirror are significantly affected by the nature and the weight of all the layers involved in the device, from the top electrode to the bottom layer of the reflector. Moreover, k_{eff}^2, which can be enlarged by improving the piezoelectric response of the AlN films, also depends critically on the thickness ratio of the electrodes and the piezoelectric layer, the nature of the electrodes and the acoustic isolation. Achieving great values of k_{eff}^2 and Q, which are essential to set the final bandwidth of the filters, requires a careful iterative design of the whole structure.

BAW-based filters operating around 2 GHz require AlN films of around 1400 nm; in this thickness range films of excellent piezoelectric properties are currently deposited on 200 mm Si wafers through optimized industrial processes. However, the thickness of the films required for 10 GHz applications decreases dangerously to around 160 nm. So far, although high frequency SMRs based on thin AlN films (from 150 nm to 300 nm) are being developed in some research institutions [1, 2], the crystal quality of such films is still far from that of thicker films, which gives rise to low k_{eff}^2 devices. As far as we know, competitive high frequency resonators with k_{eff}^2 greater than 6% have only been achieved in devices suspended over an air cavity [3, 4].

In this paper we present AlN layers with thicknesses ranging from 160 nm to 200 nm exhibiting crystalline and piezoelectric properties comparable to those of 1000 nm-thick films. AlN films are deposited by AC reactive sputtering on iridium electrodes. We investigate the effect of the pretreatment of the Ir bottom electrode and that of a two-stage deposition process that promotes the nucleation of AlN microcrystals at the beginning of the deposition process. The structure, stress, and piezoelectric response of the films are analyzed by means of standard techniques. To demonstrate the high quality of the material, SMRs at around 8 GHz are designed, fabricated and characterized.

II. Experimental Techniques

AlN films were deposited in an Endeavor-AT PVD cluster tool of OEM Group 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 500°C) using an external IR heater to warm the wafer before or during deposition.

X-ray θ/2θ diffraction patterns were recorded between 16° (θ) and 40° (θ). Rocking curves (RC) around the (00·2) AlN reflection (18.02°) and (111) Ir reflection (20.32º) were measured as well; they were fitted by Gaussian curves to obtain their FWHM. Infrared reflectance (IRR) spectra were measured with unpolarized light at an incidence angle of 30° between 200 and 4000 cm^{-1}. They allowed to assess the texture of the AlN films [5] and to obtain stress values independent of the substrate curvature. This last is important as the substrate bending is not only due to AlN stress but also to the relaxation of Ir stress; so bow measurements alone do not allow deducing the stress in the samples.

SMRs were fabricated by building Ir/AlN/Ir stacks on top of acoustic reflectors formed by five alternated layers of SiO_2 and Ir. The combination of the high acoustic impedance Ir (120×10^6 $kg/m^2\cdot s$) [6] with a specifically developed porous-SiO_2 (p-SiO_2) of low acoustic impedance (9×10^6 $kg/m^2\cdot s$) [7] provided the desired acoustic isolation. The p-SiO_2 uppermost layer of the mirror was mechanically polished to reduce roughness to less than 1 nm. This step was essential to achieve well-performing AlN layers. Ti/Mo and Ti/W seed layer were used to promote the growth of highly (111)-oriented Ir layers with narrow RC (FWHM in the range of 2.5º). Ir bottom electrodes were deposited either by e-beam evaporation at a substrate temperature of 420ºC or by pulsed DC sputtering at 350ºC. Both methods provided Ir films of similar crystal quality.

The electrical impedance of the resonators, derived from the measured reflection parameter (S_{11}), was fitted with Mason's model [8] to obtain accurate values of both material and effective electromechanical coupling factors (k_{mat}^2 and k_{eff}^2). The method allows assessing the material properties independently on the design of the device. Quality factors at resonant (Q_r) and antiresonant (Q_a) frequencies were derived from the slope of the phase of the electrical impedance.

III. Results and Discussion

A. *Setting of the deposition parameters*

In a first set of experiments, the AlN thin films were sputtered on Ir electrodes grown on oxidized Si wafers. The aim was to set the deposition conditions to obtain the best AlN films achievable (purely 00·2-oriented with narrow RC and high piezoelectric activity). A complete structural characterization was carried out using the combined film assessment described in ref. [9]. BAW resonators (with the poor acoustic isolation provided by a simple SiO_2 layer) were fabricated and characterized to asses the piezoelectric response.

Besides sputter conditions, the degree of c-axis texturing and polar orientation of AlN grains are closely related to the texture and surface roughness of the underlayer substrate. Therefore, a predeposition treatment of the substrate can significantly influence the film orientation and the piezoelectric response. The search of the best conditions for deposition of AlN on Ir bottom electrodes was based on the results obtained during process optimization of AlN on Mo electrode [10] and included investigation of the AlN crystal orientation versus in-situ predeposition treatment of the wafer and sputter process conditions. Keeping constant the earlier optimized parameters of the sputter system (such as magnetic field configuration, AC cathode power, and Ar and N_2 gas flows), we varied RF power and duration of the RF plasma etch process and wafer temperature during deposition. Additionally, different deposition procedures were investigated, which included a predeposition annealing in vacuum and a two-step deposition process with variation of the sputter parameters in the middle of the process.

Ion bombardment from RF discharge near the substrate has the objectives to clean and activate the surface of the Ir electrode right before AlN deposition. The intensity (energy and duration) of the ionic bombardment has to be adjusted carefully because too low or too high values tend to worsen the piezoelectric response of AlN owing presumably to the generation of inversely polarized microcrystals. We found that etch with RF power 70 W and Ar pressure 5×10^{-3} Torr for 60 s ensures the best conditions for formation of highly oriented films with good piezoelectric response.

Two-step deposition consists in the use of a higher temperature of about 400-450˚C and higher nitrogen gas flow enabling operation of the S-Gun magnetron in a "deep" poison mode at the first stage of process (first 50 nm-thick film) to facilitate the nucleation. In a second step, the remaining film is deposited at a wafer temperature of about 300-350˚C without external heating and the N_2 flux is reduced to the value enabling the magnetron discharge to remain in a poison mode, but at the work point located closer to a transition zone between a poison and a metallic mode on the hysteresis curve [11]. Experiments have shown that a permanent wafer heating at 400 °C during the entire process does not improve remarkably the crystal orientation, indicating that higher adatom mobility is required mostly at the nucleation stage ensuring formation of grains with less structural defects.

Residual stress in AlN films deposited by the S-Gun is well controlled by varying the Ar gas flow (Ar gas pressure). Films deposited with relatively low pressure typically have compressive stress. Increasing the pressure reduces compressive stress or can convert it to tensile. However, due to the fact that deposition rate and film thickness uniformity depend on gas pressure too, stress control by means of sputter gas regulation has limited applicability. Therefore, the S-Gun is equipped with a special unit ensuring fine stress tuning in the AlN films independently on other film and process parameters. The technique is based on manipulating the compressive stress in the films by controllably suppressing the flux of charged particles from AC discharge to the substrate by redistributing the discharge current between the Al targets and the internal shields of the magnetron [12]. A reduction of this bombardment leads to lower compressive (or higher tensile) stress in the film if required. With this method the stress of AlN on Ir can be set from strongly tensile (+1000 MPa) to strongly compressive (-1000 MPa). Most of the films deposited for this study had reproducible tensile stress below 200 MPa.

A parameter that strongly affects the quality of the AlN layer is the texture of the bottom electrode, which is measured through width of the RC around the (111) Ir peak. A wide RC around the (111) Ir peak can be associated either to a bad crystal quality of the Ir layer or to the growth of well-oriented grains on a rough substrates. Fig. 1 shows the variation of the RC around the (00·2) AlN peak and k_{mat}^2 as a function of RC around the (111) Ir peak. For identical deposition conditions and seed layers, the RC can vary from 20º to 2.4º as the roughness of the substrate varies from 20 nm to below 1 nm. AlN films grown on well-textured Ir layers have narrow RCs and high k_{mat}^2 values. Even on Ir underlayers with a relatively wide RC of 5º, AlN films deposited using optimized sputter conditions show a RC width lower than 3º and present high values of k_{mat}^2 of up to 6.7%. However, when rough substrates were used the width of the Ir (111) RC increases to around 19º and the AlN RC increases up to 12º, but the material coupling factor drops only slightly to around 5.4%. This is due to a "geometrical" widening of the AlN RC and not to a worsening of the crystalline structure of the microcrystals.

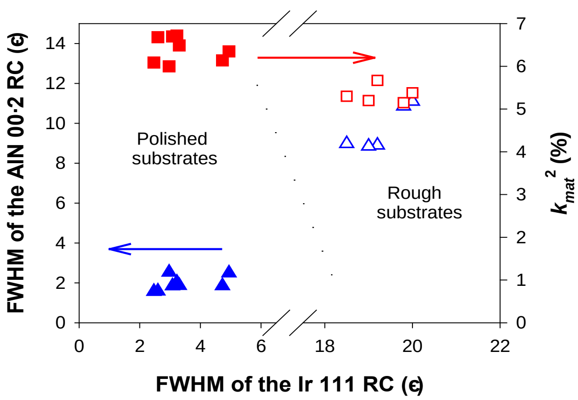

Figure 1. RC around the (00·2) AlN XRD peak (▲) and k_{mat}^2 (■) as a function of the RC around the (111) Ir peak.

It was found that it is possible to produce highly oriented AlN films even on Ir electrodes having essentially different quality. The best achievements at this stage were AlN films 200 nm-thick with a RC 1.6° wide grown on Ir with RC width of the 111 peak of 3.8°. For comparison, a 1 µm-thick film deposited under the same deposition conditions exhibited RCs of 1.27°. These results are comparable and even better than those obtained for 200 nm and 1 µm thick AlN films deposited on prime quality Si wafers.

Figure 2 shows two images obtained by scanning electron microscopy of a well-oriented 200 nm-thick AlN film on an Ir underlayer. A clear columnar structure formed by grains with a basal diameter of around 40 nm can be appreciated.

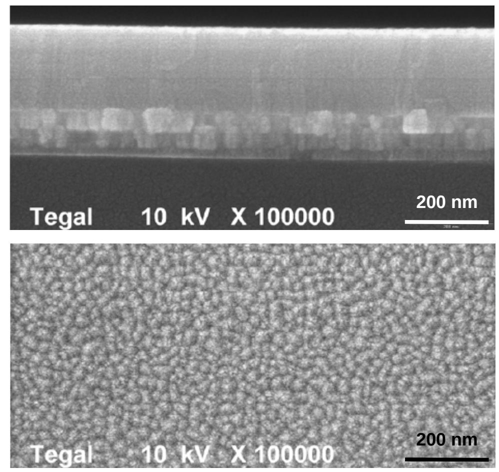

Figure 2. Cross-section and plane-view SEM images of a typical 200 nm-tick AlN film.

In summary, the structural characterization demonstrated that the best performing AlN films were achieved with the following conditions: in-situ wafer annealing in vacuum, low-power RF plasma etch in the PRF module, and 2-step AlN deposition at elevated temperature.

B. High frequency resonators

To demonstrate the viability of the AlN films for high frequency filter applications, SMRs operating around 8 GHz were designed and fabricated. Acoustic reflectors made of five alternated layers of p-SiO2 and Ir were designed to obtain an acoustic transmittance of the longitudinal resonant mode lower than -35 dB in a wide frequency band that includes the resonant frequency and, simultaneously, an acoustic transmittance of the shear modes lower than -20 dB. This was achieved by setting the thickness of some layers in the mirror to values different from λ/4, according to [13]. This design improves the acoustic isolation at the resonant frequency, which increases the quality factor of the SMR compared to that obtained on conventional symmetric λ/4 Bragg mirrors. Once the acoustic reflector was designed and tuned to the desired resonance frequency, a simulation of the frequency response of the SMRs was performed in order to obtain the thickness of the layers composing the piezoelectric stack (AlN and Ir electrodes) that would maximize the value of the k_{eff}^2. To simplify the problem the top and bottom electrode were considered of identical thickness. Figure 3 shows the simulation performed by varying the electrode thickness. Although all the piezoelectric stacks shown in figure 3 produce a resonance at 8 GHz, the maximum value of k_{eff}^2 is achieved for a unique combination of thicknesses, which corresponds to AlN layer 260 nm-thick sandwiched between two Ir electrodes 45 nm-thick.

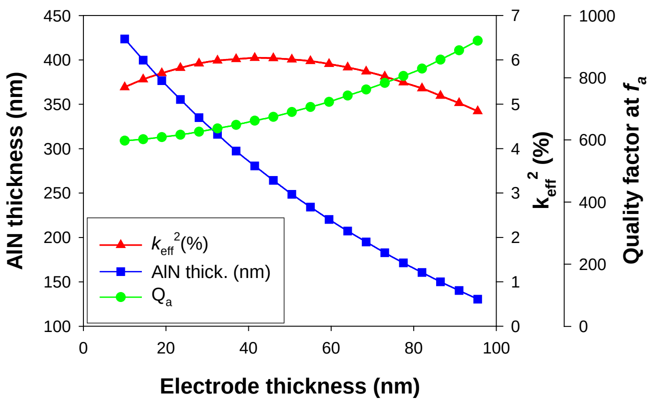

Figure 3. AlN thickness (■), k_{eff}^2 (▲), and Q_a (●) vs Ir bottom electrode thickness. Simulations were made for resonators tuned at 8 GHz and AlN layers with k_{mat}^2 of 6.5%. Acosutic losses in AlN were considered.

One of the main problems of high frequency resonators is the use of very thin electrodes that increases the series resistance reducing the value of Q_r. The situation gets worse when using high density metals like Ir, which imposes a severe reduction of the layer thickness in order to keep the resonant frequency constant. On the other hand, Q_a mainly depends on the acoustic losses through the materials of the whole structure. To achieve the best design a compromise has to be reached between the values of k_{eff}^2 and Q. Therefore, we have considered that 75 nm-thick Ir electrodes yielding series resistances around 1 Ω and Q_r of 150 are acceptable values.

Figure 4 shows the frequency measurements of a typical SMR tuned at 8 GHz; for this device we obtained k_{eff}^2=5.8%, Q_r =160 and a Q_a=930. The k_{mat}^2 required to fit the frequency response of this device with Mason's model was 6.7%. These results show that although the AlN films are of very good quality, the design of the piezoelectric stack can be improved. A reduction of the series resistance is mandatory, which could be achieved by using a metallic layer of a low density material, such as Al or Ti, under the Ir bottom electrode. This could increase the value of k_{eff}^2 while keeping good values of Q_r.

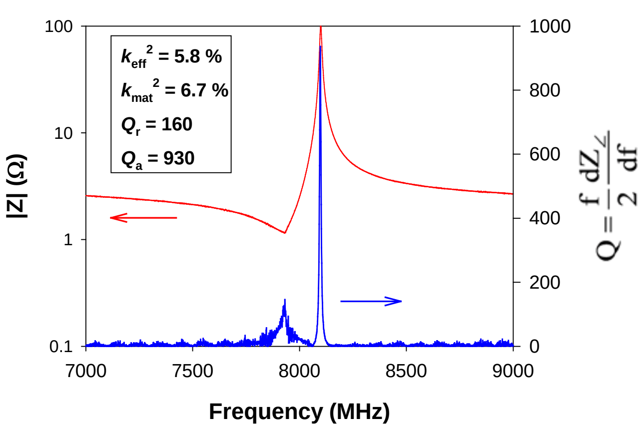

Figure 4. Impedance modulus and Q as a function of frequency.

IV. Conclusions

AlN films with thicknesses as low as 160 nm have been grown on Ir electrodes for fabricating 8 GHz SMRs. These very thin films have structural and piezoelectric properties similar as the best obtained for 1 µm-thick films. SMRs tuned at 8 GHz show very good values of k_{eff}^2 and Q_a. New designs allowing to reduce the series resistance of the electrodes are required to improve Q_r.

Acknowledgement

This work has been supported by Ministerio de Educación y Ciencia of Spain through projects MAT2007-62162, Comunidad de Madrid and UPM through the IV PRICIT Programme (Q060940109), and through the European Regional Development Fund (FEDER).

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