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Fabrication of piezoelectric AlN thin film for FBARs

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This paper focuses on the fabrication of film bulk acoustic-wave resonator (FBAR) comprising an aluminum nitride (AlN) piezoelectric thin film sandwiched between two metal electrodes and located on a silicon substrate with a low-stress silicon nitride (Si_3N_4) support membrane for high frequency wireless applications, and analyzes the optimization of the thin AlN film deposition parameters on Mo electrodes using the reactive RF magnetron sputter system. Several critical parameters of the sputtering process such as RF power and Ar/N_2 flow rate ratio were studied to clarify their effects on different electrodes characteristics of the AlN films. The experiment indicated that the process for Mo electrode was easier compared with that of the Pt/Ti or Au/Cr bi-layer electrode as it entailed only one photo resist and metal deposition step. Besides, Pt/Ti or Au/Cr electrodes reduced the resonance frequency due to their high mass density and low bulk acoustic velocity. Compared with the case of the Al bottom electrode, there is no evident amorphous layer between the Mo bottom electrode and the deposited AlN film. The characteristics of the FBAR devices depend not only upon the thickness and quality of the AlN film, but also upon the thickness of the top electrode and the materials used. The results indicate that decreasing the thickness of either the AlN film or the top electrode increases the resonance frequency. This suggests the potential of tuning the performance of the FBAR device by carefully controlling AlN film thickness. Besides, increasing either the thickness of the AlN film or higher RF power has improved a stronger *c*-axis orientation and tended to promote a narrower rocking curve full-width at half-maximum (FWHM), but increased both the grain size and the surface roughness. An FBAR device fabricated under optimal AlN deposition parameters has demonstrated the effective electromechanical coupling coefficient (k^2_{eff}) and the quality factor (Q_{f_x}) are about 1.5% and 332, respectively.

sputtering, thin film, piezoelectric

The rapid growth of wireless mobile telecommunication systems has led to an increasing demand for high-frequency oscillators, filters and duplexers capable of operating in the 0.5 to 5 GHz frequency range. Conventionally, microwave ceramic resonators and surface acoustic wave (SAW) resonators have been applied in this frequency range. However, microwave ceramic resonators tend to be physically bulky, while SAW resonators demonstrate a relatively poor sensitivity to temperature and have high insertion losses and limited power handling characteristics. Moreover, SAW devices must be generally interfaced at the board level rather than directly at the chip level. Micromachined thin film bulk acoustic-wave resonators (FBARs) have been developed to address the limitations of these conventional devices. Compared with microwave ceramic resonators and SAW resonators, FBAR devices have the advantages of low cost and enhanced electrical performance, and are characterized by low insertion losses, high power handling capabilities and high frequency operation[1−3]. Furthermore, the miniature scale of FBARs and the possibility of mounting them on Si or GaAs substrates permit their use within microwave monolithic

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integrated circuits (MMICs)[4].

The performance of the FBAR device depends upon the presence of a large acoustic impedance mismatch on both sides of the piezoelectric material in order to trap energy and hence produce resonating characteristics. This requires either the use of a Bragg reflector on the lower side of the piezoelectric[5], or the inclusion of an air/crystal interface beneath the resonator.

AlN is preferred over ZnO as the piezoelectric material since it has a superior compatibility with silicon[6], a higher bulk acoustic wave velocity, higher electrical resistivity, lower mass density and a wider band gap. Although previous studies have generally adopted Pt/Ti, Au/Cr or Al as the bottom electrode of the FBAR device, the present study deliberately specifies the use of molybdenum on account of its low resistivity, large acoustic velocity and excellent adhesive properties with the low-stress silicon nitride (Si_3N_4) supporting membrane. Consequently, this study investigates the influence of the RF power and nitrogen flow rate ratio on the deposition of highly *c*-axis oriented AlN films on Mo bottom electrodes, and studies the performance of these films for use in FBAR resonator applications.

1 Experimental procedure

Figure 1 presents a schematic illustration of a micromachined FBAR device fabricated on a (100) crystallographic oriented silicon wafer (4 inch) with a highly boron-doped layer. In the fabrication process, the substrate was initially cleaned using an RCA cleaning operation, and then a low pressure chemical vapor deposition (LPCVD) process was employed to deposit films of low-stress silicon nitride on either side of the substrate. The deposition parameters of process temperature, pressure and flow rate ratio of SiH_2Cl_2 (dichlorosilane)/NH_3 (ammonia) were kept constant at 835℃, 170 mTorr and 95/19, respectively. The two low-stress Si_3N_4 layers serve as a support membrane for the FBAR cantilever and as an etching mask, respectively. Finally, the underside of the silicon substrate was removed in a wet etching process to create a cavity under the piezoelectric-active area.

An etchant concentration of 40% potassium hydroxide (KOH) with 30% of water at 80℃ was utilized to etch the silicon substrate to an appropriate thickness. The etching rate along the (100) plane was approximately 0.9 μm/min. A 1000 Å-thick molybdenum film was deposited by DC sputter over the membrane layer and patterned using conventional photolithography techniques to form the bottom electrode. The deposition parameters of Mo electrode such as discharge power, substrate temperature, Ar-flow rate, deposited pressure and deposited rate were 150 W, 50℃, 24 sccm, 3.2×10^{-6} Torr and 0.36 Å/s, respectively. Subsequently, the reactive RF magnetron sputtering process was employed to deposit a thin AlN film on top of the molybdenum layer. Finally, an aluminum film was sputter deposited over the AlN film and patterned photolithographically to form the top electrode. The detailed deposition of RF sputtering parameters for AlN films is summarized in Table 1.

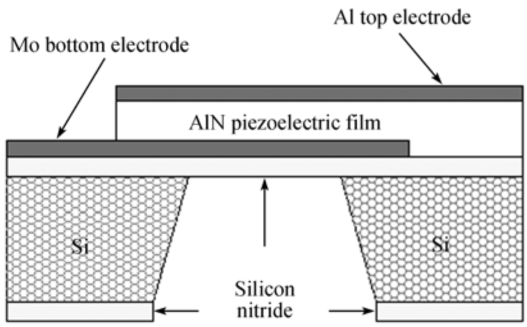

Figure 1 Cross-sectional view of FBAR.

Table 1 Parameters used for deposition of AlN thin films

Parameters	AlN Film
Target	Al (99.999%)
Substrate	$Mo/Si_3N_4/Si$
Substrate-to-target distance	50 mm
Substrate temperature	250℃
Base pressure	1×10^{-6} Torr
Sputtering pressure	5×10^{-3} Torr
RF power (Watts)	200, 300, 400, 450
Gas flow rate ratio (sccm)	Ar/N_2=5/7, Ar/N_2=4/8, Ar/N_2=3/9, Ar/N_2=2/10

The present study has two principal objectives, namely to investigate the growth of piezoelectric AlN films and to study the characteristics and performance of FBAR devices incorporating these films. In order to study the quality of thin AlN films, 1000 Å thick Mo films were sputtered over low stress silicon nitride films deposited on silicon wafer substrates. Subsequently, thin AlN films were deposited using a reactive RF magnetron sputtering method under various sputtering parameters, i.e. RF powers of 200, 300, 400 and 450 W, and various nitrogen flow rate ratios ($N_2/(Ar+N_2)$) of 58%, 66%, 75% and 83%, while all the other parameters were kept constant.

In investigating the deposited AlN films, this study focuses principally on the preferred orientation and surface roughness of the films since these characteristics are known to have significant impacts on the resonance properties and reliability of FBAR devices. The crystalline structure and crystallographic orientation of each AlN film were analyzed by X-ray diffraction (XRD, RIGAKU D/max 2.B) analysis with Cu*Kα* radiation (λ = 1.5418 Å). The power of the XRD was fixed at 25 kV and 5 mA, and scanned from 30° to 50° at a scanning speed of 4°/min. The cross-sectional of the various AlN film grain structures were observed using scanning electron microscope (SEM, PHILIPS XL-40FEG). Furthermore, atomic force microscope (AFM, SPA300HV) was utilized to facilitate a detailed analysis of the surface morphology and surface roughness of each of the AlN films. The AFM analysis was carried out in contact mode using a scan size area of 2 μm^2. The thickness of the various films was determined using a stylus profilometer (Veeco DEKTAK). Finally, the *S* parameters were measured by a network analyzer (HP 8722ES) and a wafer probe station (Cascade Microtech).

2 Results and discussion

In order to study the feasibility of tuning the RF power to obtain highly *c*-axis oriented AlN films, the present study developed AlN films under RF powers of 200, 300, 400 and 450 W, respectively. Figure 2 presents the XRD patterns of the corresponding AlN films prepared at a sputtering pressure of 5 mTorr and a nitrogen flow rate ratio of 75%. It is noted that in each case, the AlN film thickness is approximately 2.7 μm and that the film was deposited over a period of 3 h.

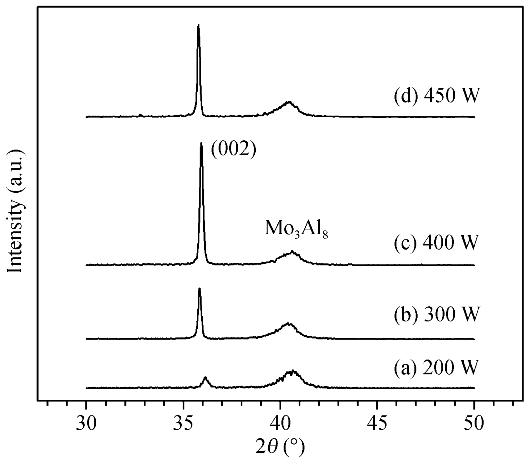

Figure 2 XRD patterns of AlN films on Mo deposited at different RF powers. (a) 200 W; (b) 300 W; (c) 400 W; (d) 450 W.

Figure 2(a) shows the XRD pattern of the AlN film deposited under an RF power of 200 W. It is observed that the diffraction intensity of the (002) peak is relatively weak compared with that of the Mo_3Al_8. This suggests that the *c*-axis of the AlN film is approximately parallel to the substrate surface. Meanwhile, Figure 2(b) indicates that increasing the RF power to 300 W causes the intensity of the (002) peak to become relatively stronger than that of the Mo_3Al_8. As the RF power is further increased to 400 W (Figure 2(c)), it is clear that there is a significant increase in the intensity of the (002) peak, indicating that the *c*-axis of the hexagonal AlN structure is perpendicular to the substrate surface. Testing revealed that increasing the RF power further to 450 W shown in Figure 2(d) failed to yield any further improvement in the intensity of the (002) peak. Hence, the RF power was fixed at 400 W throughout the remainder of the study.

Figure 3 shows the relationship of different RF powers between the AlN film thickness and the AlN full width at half maximum (FWHM). Increasing either the RF sputtering power or the thickness of the AlN film improves the *c*-axis orientation of the film and promotes a narrower FWHM.

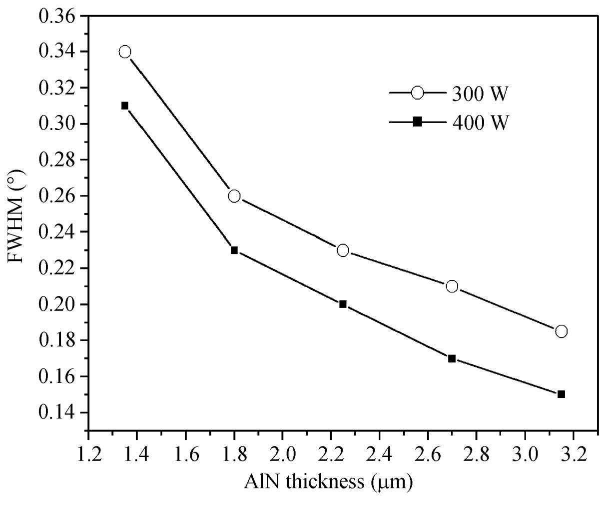

Figure 3 Relationship between the AlN film thickness and FWHM of the (002) peak of AlN films with different RF powers grown on Mo bottom electrode.

The experimental results presented in Figures 2 and 3 confirm that AlN films deposited on the Mo bottom electrode prepared under a RF power of 400 W have a stronger diffraction intensity of the (002) peak than those prepared under lower RF power conditions (200 W, 300 W) or higher RF power of 450 W. These results can be explained by assuming the basal plane in hexagonal structures to possess the lowest surface energy and the maximum atomic density. Increasing the RF power not only enhances the sputtering yield, but also increases the kinetic energy of the particles in the plasma. Consequently, the aluminum-nitride complex particles have sufficient kinetic energy to attach themselves to the substrate, hence providing the adatoms with increased opportunities to move to the lowest energy state and to form a highly *c*-axis-oriented crystalline film structure. However, when the RF power exceeds 400 W, the kinetic energies of the secondary atoms will also increase. These high-energy atoms then attack the substrate surface, causing surface damage and prompting deterioration in the preferred *c*-axis orientation as shown in Figure 2(d)[7]. As described above, the specification of a 400 W RF power yields AlN films on Mo bottom electrode is improved with the preferred *c*-axis orientation in our experiment.

In order to study the effects of the nitrogen flow rate ratio on the crystallographic orientation of the AlN films, Figure 4 shows the corresponding XRD results of the AlN films deposited on Mo electrode at nitrogen flow rate ratios of 58%, 66%, 75% and 83%, with a power of 400 W and a sputtering pressure of 5 mTorr.

It is evident that the crystalline structures of these films are all *c*-axis-oriented and hexagonal. Furthermore, increasing the N_2 flow rate ratio to 75% shown in Figure 4(c) causes the AlN film to develop a stronger preference for the preferred (002) orientation, as the atomic bombardment of the film surface causes an increase in the film density. Under bombardment, the kinetic energy of the surface atoms is increased and sufficient for some of these atoms to rearrange themselves to achieve thermal equilibrium conditions, hence reducing the voided regions within the microstructure. The flux of the bombarding particles increases as the nitrogen flow rate ratio increases. Therefore, the adatomic mobility at the film surface is also improved as a result of the increase in energy transfer taking place at the film surface. Consequently, an elevated nitrogen flow rate ratios are beneficial in developing AlN films with the desired normal orientation and hence to manifest enhanced piezoelectric qualities. Further increase nitrogen flow rate ratios to 83% shown in Figure 4(d) failed to yield any further improvement in the intensity of the (002) peak. Hence, the nitrogen flow rate ratios were fixed at 75% through

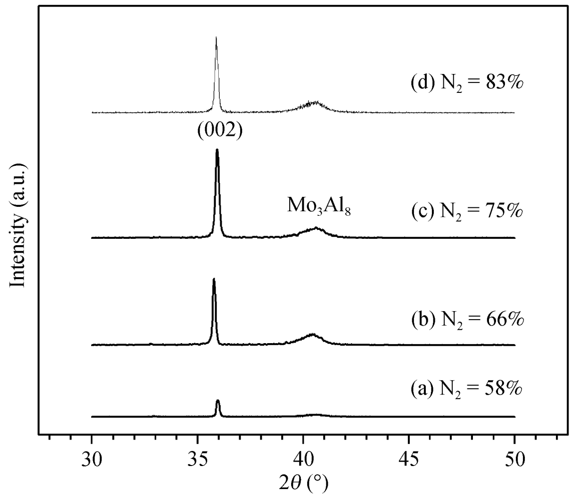

Figure 4 XRD patterns of AlN films on Mo deposited at various nitrogen flows rate ratios. (a) N_2=58%; (b) N_2=66%; (c) N_2=75%; (d) N_2=83%.

out the remainder of the study.

Figure 5 shows the FWHM of the (002) peak of AlN films grown on Mo bottom electrode as a function of the nitrogen flow rate. The smaller FWHM of the (002) peak of AlN film was 0.17° at nitrogen flow rate of 75%, while increasing the nitrogen flow rate to 83% cause the larger FWHM of 0.175°.

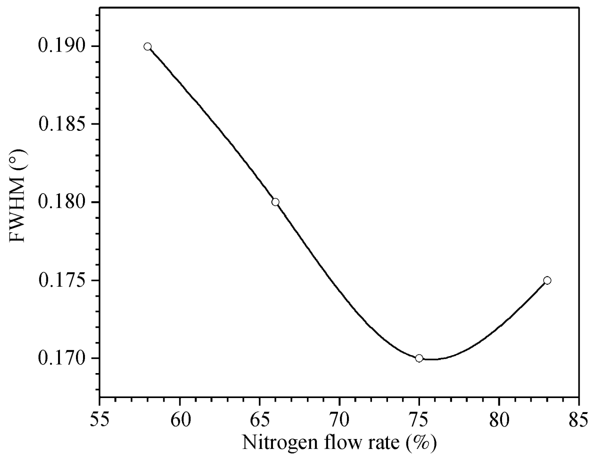

Figure 5 FWHM of the (002) peak of AlN films grown on Mo bottom electrode as a function of the nitrogen flow rate.

Figure 6(a) and (b) present the SEM micrographs of the cross-sectional structure of AlN films deposited at RF powers of 300 and 400 W, respectively, with N_2 flow rate ratios of 75% and sputtering pressures of 5 mTorr. The typical columnar structure with tapered tops associated with the growth of AlN films on Mo electrodes is particularly evident in 400 W RF power case shown in Figure 6(b). The microstructures of the deposited films are not homogeneous and are seen to have fine grain structures in the vicinity of the substrate surface. The columnar structures clearly develop as the film thickness increases. This characteristic of the AlN-Mo interface ensures good adhesion properties between the two layers, and is indicative of a smooth interfacial quality in fabricated FBAR devices.

The surface roughness of each film was measured using an AFM technique. Figure 7 presents the statistical analysis of the surface roughness of AlN films prepared at various RF powers using an N_2 flow rate ratio of 75%. Figure 7(a) presents the surface roughness of the films prepared at 300 W, showing an equivalent 3-D view with z-axis of 150 nm. It can be seen that the average roughness (R_a) is 14 nm and that the average peak to the valley height of each grain column is 116 nm. Meanwhile, Figure 7(b) shows the surface roughness of the AlN films prepared at 400 W. The average roughness of these films is seen to be 4 nm, while the average peak to valley height of each grain column is 30 nm. It is observed that the films prepared at 400 W have a very smooth upper surface. Therefore, it would appear that smaller grain columns are associated with a smoother upper surface. The results of Figure 7 indicate that preparing AlN films at RF power of 400 W and N_2 flow rate ratio of 75% not only refines the film grain size, but also yields uniform films with smooth morphologies, and hence improves the coupling factor when these films are utilized in FBAR devices.

In general, the choice of electrode material also has a pronounced influence upon the performance of an FBAR device. It is of particular importance to consider the longitudinal velocity and the mass density of the specified electrode material. Figure 8 shows the experimental results for both the resonance frequency obtained with Mo and Pt/Ti bottom electrodes with various AlN film thicknesses of 2.25, 2.7, 3.15 and 3.6 μm, while the thickness of Si_3N_4 membrane, bottom and top electrode was kept constant of 0.2, 0.1 and 0.18 μm, respectively. It can be seen that the smaller mass loading effect and larger acoustic velocity associated with Mo electrodes result in an improved FBAR resonance frequency compared to the cases of Pt/Ti electrodes are employed. It is also observed that the resonance frequency of the FBAR is strongly affected by the thickness of the AlN film layer. Specifically, reducing the AlN thickness yields a

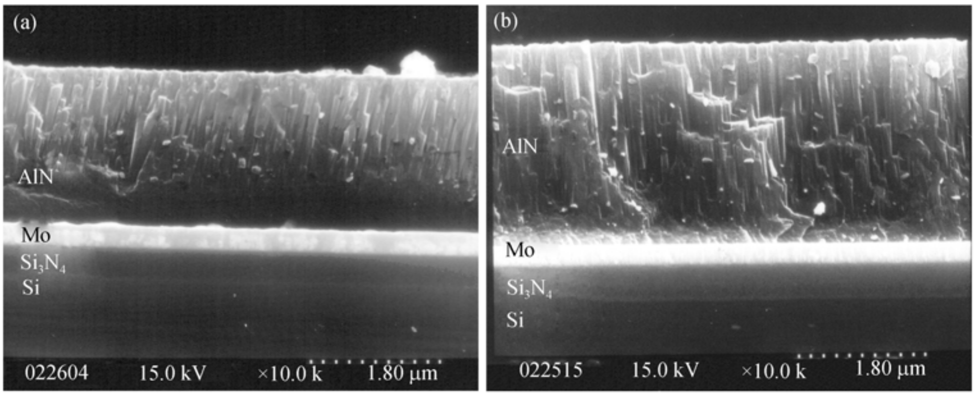

Figure 6 Cross-sectional SEM of AlN films on Mo bottom electrode at various RF powers. (a) 300 W; (b) 400 W.

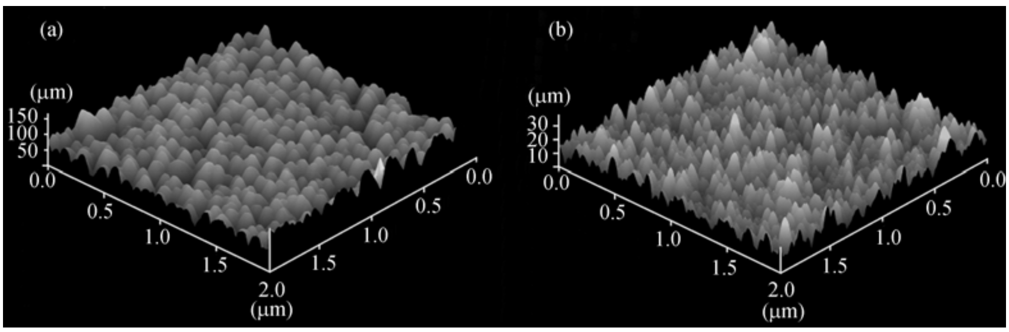

Figure 7 AFM surface roughness of AlN film deposited on Mo at various RF powers. (a) 3-D view of 300 W with z-axis of 150 nm; (b) 3-D view of 400 W with z-axis of 30 nm.

significant increase in the resonance frequency since the thickness field excitation of the FBAR is reduced, thereby shortening the acoustic path. The results of Figure 8 demonstrate that, subjected to a minimum practical thickness, FBARs can be designed to operate at different resonance frequencies by carefully controlling the thickness of the deposited AlN film.

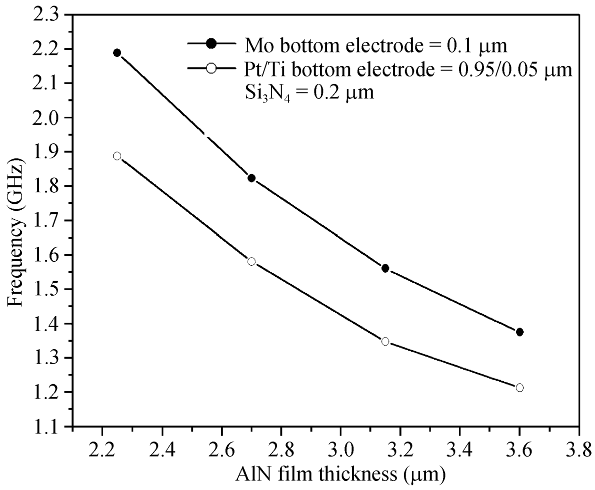

Figure 8 The resonance frequency obtained with Mo and Pt/Ti bottom electrodes with various AlN film thicknesses.

In order to test the performance of the AlN film in FBAR devices, a two-port FBAR device with a four-layered composite structure was implemented and tested. Figure 9 shows the SEM image of top view of fabricated two-port AlN FBAR, and its piezoelectric-active area was square shape with 150 μm×100 μm measured by G-S-G probe, the thickness of low stress Si_3N_4, AlN film, Mo (bottom) and Al (top) electrodes was consisted of 0.2, 2.25, 0.1 and 0.18 μm, respectively.

The impedance characteristic of the fabricated two-port AlN FBAR is shown in Figure 10. The parallel and series resonance frequencies of the FBAR appeared at 2.19 and 2.18 GHz, respectively.

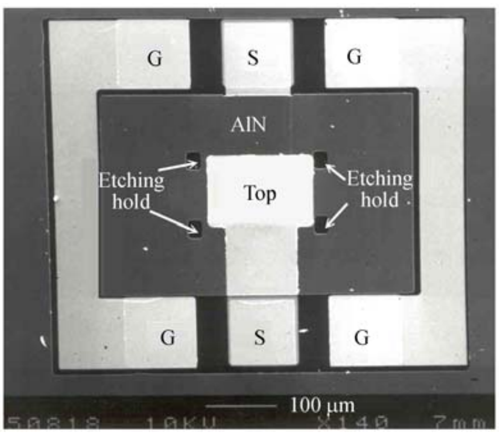

Figure 9 SEM image of top view of fabricated two-port FBAR.

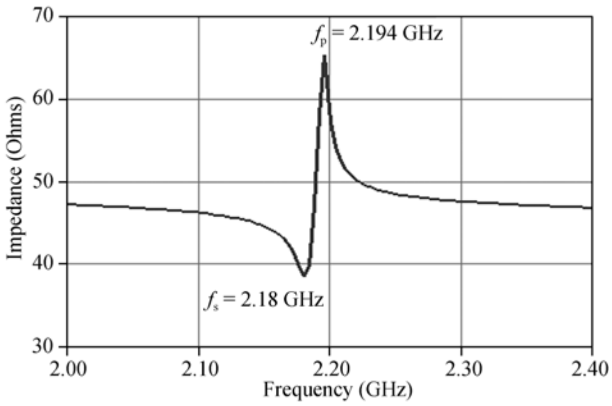

Figure 10 Input impedance versus frequency of the fabricated two-port AlN FBAR.

The effective electromechanical coupling coefficient (k^2_{eff}) and the quality factor (Q_{f_x}) determine the piezoelectric quality of the AlN film. From the measured frequency response of two-port AlN FBAR, we calculated the k^2_{eff} and Q_{f_x} using the following equations:

$$k^2_{\mathrm{eff}} = \frac{\left(\frac{\pi}{2}\right)\left(\frac{f_s}{f_p}\right)}{\tan\left(\left(\frac{\pi}{2}\right)\left(\frac{f_s}{f_p}\right)\right)} \approx \left(\frac{\pi}{2}\right)^2 \frac{f_p - f_s}{f_p}, \tag{1}$$

$$Q_{f_x} = \frac{f_x}{2}\left|\frac{\mathrm{d}\angle Z_{\mathrm{in}}}{\mathrm{d}f}\right|_{f_x}, \tag{2}$$

where $\angle Z_{\mathrm{in}}$ is the phase response expressed in radians and f_x corresponds to either parallel (f_p) or series (f_s) resonant frequencies of the two-port AlN FBAR device. The k^2_{eff} and Q_{f_x} were about 1.5% and 332, respectively.

3 Conclusion

This study employed the reactive RF magnetron sputtering method to deposit highly *c*-axis-oriented fine polycrystalline AlN films on Mo electrodes. The results show that AlN films prepared at the RF power of 400 W and an increased N_2 flow rate ratio of 75% demonstrate a stronger tendency toward the preferred *c*-axis orientation and exhibit smoother morphologies. Hence, these films enhance the coupling factor when they were applied in FBAR devices. Moreover, it is shown that increasing either the thickness of the AlN film or the intensity of the 400 W RF power tends to promote a narrower FWHM.

An FBAR device fabricated under optimal AlN deposition parameters has demonstrated the k_{eff}^2 and the Q_{f_x} were about 1.5% and 332, respectively. The present results suggest the potential to tune the resonance frequencies of FBAR devices by carefully controlling the thickness of the AlN layers during the fabrication process. for it is related both to the quality and the thickness of the AlN.

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