Proceedings of the 2003 IEEE International Frequency Control Symposium and PDA Exhibition
Jointly with the 17th European Frequency and Time Forum

Experimental and Theoretical Investigation on the Relationship between AlN Properties and AlN-based FBAR Characteristics

Jun-Phil JUNG, Jin-Bock LEE, Myung-Ho LEE, and Jin-Seok PARK

Dept. of Electrical Engineering, Hanyang University

1271 Sa-1 dong, Sangrok-ku, Ansan, Kyonggi-do 426-791, South Korea

Abstract - Film bulk acoustic resonators (FBARs) with an Al/AlN/Mo/Si (111) configuration are fabricated. In particular, the effects of deposition conditions on material properties of AlN films grown on Mo/Si substrate as well as the performance of FBARs are studied. Piezoelectric AlN films are deposited using RF magnetron sputtering at RF power = 250 W ~ 600 W, N_2/Ar ratio = 5/25 ~ 25/5, working pressure = 5 mTorr, substrate temperature = 250 ^oC. For all the deposited AlN films, the x-ray diffraction (XRD) spectra and full width at half maximum (FWHM) of rocking curves are measured in terms of the deposition conditions, to characterize the c-axis preferred orientation and crystal quality. The frequency response characteristics (S_{11}) of the fabricated FBARs are also measured. The experimental results indicate that the characteristics of FBARs can be determined by the material properties of the AlN films. Furthermore, the theoretical relation ship between the impedance parameters (R_m) of the BVD model and the AlN properties has been established.

I. Introduction

Wireless networks are growing rapidly in the frequency range from 500 MHz to 6 GHz. These systems include pager, cellular, navigation, satellite communication, and various forms of data communication. Within subsystems, miniaturization of RF components is needed to accommodate increased levels of circuit complexity. In addition, newer architectures require higher performance frequency control components. Ceramic resonator technology is able to meet these requirements, but with a component about the same size as a cigarette filter. Surface acoustic wave (SAW) devices can reduce the size considerably, but poor electrical performance has required a split-band approach using switches to select the upper half-band or lower half-bands. However, FBARs are capable of overcoming these problems.

Practical film bulk acoustic resonators (FBARs) consist of a piezoelectric thin film sandwiched between top and bottom electrodes onto which an electrical field is then applied [1,2]. Thin film AlN is one of the promising piezoelectric materials for FBARs. A widely-utilized form of the piezoelectric AlN layer is sputtered-polycrystalline rather than epitaxial since the epitaxial AlN may not be economically feasible with present technology. The nature of polycrystalline AlN is determined by the bottom electrode as well as the film deposition condition [3]. Therefore, deposition parameters are usually adjusted to provide columnar growth of the AlN layer and the selection of proper bottom electrode is important as well. When polycrystalline AlN films are used in FBARs, the electro-acoustic coupling coefficient (k_t^2) strongly depends on the film quality. The k_t^2 value must be known as an important material parameter in the electrical analysis of FBARs since the k_t^2 parameter affects the impedance of the resonator and thus alters the whole frequency response characteristics of the FBARs. The Butterworth-Van Dyke (BVD) model is one of the widely used equivalent circuits for a piezoelectric resonator. Recently, the modified BVD circuit, which consists of six electrical elements, has also been suggested to provide more accurate fitting data [4,5]. However, in these models the variation of resonator impedance due to the change of AlN property can hardly be taken into consideration.

The purpose of this research is to experimentally investigate the influence of material properties of piezoelectric AlN layer on device characteristics of AlN-based FBARs, and moreover, to provide a theoretical relationship for formulating the impedance of resonator as a function of material parameters.

II. Experimental

Thin films of AlN were deposited on Si(111) by a widely-utilized RF reactive magnetron sputtering method. The Al target (99.999% in purity) was sputtered using a high purity Ar and N_2 gas mixture. During deposition, the substrate was rotated at a low speed of 5 rev/min for enhancing the thickness uniformity of deposited films. Mo films were deposited on Si(111) substrate by using the same sputtering system at the nominal condition of RF power at 600 W, working pressure at 15 mTorr, Ar at 20 sccm, and substrate temperature at RT. To examine the effect of deposition condition on properties of AlN films deposited on Mo, RF power, N_2/Ar ratio, and working pressure were varied. The detailed process conditions used to deposited the AlN, Mo, and W films are listed in Table 1.

The crystal orientations including the c-axis preferred (002)-orientation of deposited AlN films were analyzed by x-ray diffraction (XRD, Bede D3 system) and scanning electron microscopy (SEM), from which the texture coefficient (TC) for the (002)-orientation reflecting the piezoelectric property was estimated.

The crystal quality of those films was also characterized both by the $\theta - 2\theta$ scans obtained from XRD spectra and by the full-width at half maximum (FWHM) estimated from rocking curves [6]. The RMS surface roughness of AlN films were also extracted from atomic force microscopy (AFM, Auto-Probe CP, PARK Scientific Instruments) topographies.

FBARs with Al/AlN/Mo/Si configuration (over-moded type) were fabricated to estimate the effect of material properties of AlN films on device characteristics of AlN-based FBARs. Top electrodes (Al, 200 nm) was formed with a resonance area of 200 μm^2 by using a lift-off method. The frequency response was measured by a network analyzer (HP 8720C) connected to a probe station (G-S-G type), in terms of material properties of the AlN film. From the frequency response, the theoretical relationship for formulating the impedance of resonator was established as a function of material parameters.

Table 1. The deposition conditions for AlN, Mo, and W films

Conditions	AlN	Mo	W
RF power	250 ~ 600 W	600 W	700 W
Pressure	5 ~ 20 mTorr	15 mTorr	15 mTorr
Gas ratio	N_2/Ar ratio = 5/25 ~ 25/5	Ar = 20 sccm	Ar = 20 sccm
Temperature	250 ^{o}C	RT	RT

III. Results And Discussion

A. AlN films deposited on various substrates

The XRD spectra and rocking curves were measured to examine the crystal orientation and quality of AlN films deposited on various substrates. Fig. 1(a) ~ (c) shows the XRD spectra for AlN/Si, AlN/Mo/Si, and AlN/W/Si samples and the corresponding rocking curves, respectively. As viewed in Fig. 1, the films of AlN deposited on Si(111) without using metal layers exhibited only (002)-orientation, indicating the growth along the the c-axis. For the films of both AlN/Mo/Si and AlN/W/Si films, other orientations like (101) as well as (002)-orientation were observed. It should be noted that the deposited films of AlN/Si have exhibited a highly c-axis preferred orientation (i.e, the texture coefficient for (002)-orientation ≈ 100%).

The FWHM value (10.62^{o}) obtained from the AlN/Mo/Si film was observed to be much larger than that obtained from the AlN/Si film (3.81^{o}) and that of the AlN/W/Si film was not estimated. It was considered that the poor AlN films quality was attributed to the large RMS surface roughness of metal layers (Mo, W) [3]. It also should be noted that the AlN films deposited on Mo/Si layer revealed a smaller FWHM value, compared to the films deposited on the W/Si layer.

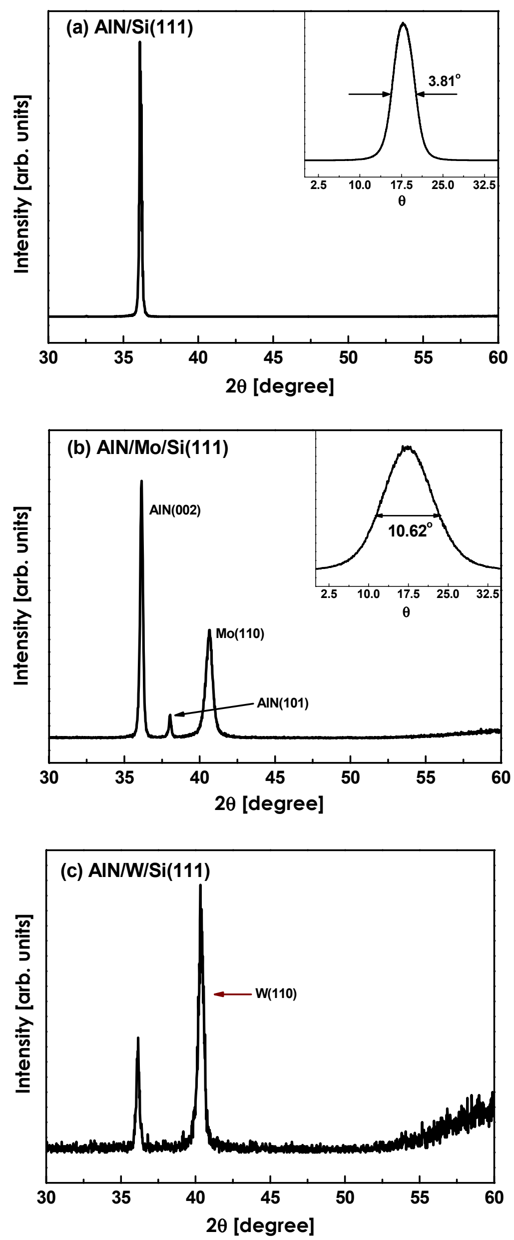

Figure 1. X-ray diffraction peaks and FWHM values of rocking curves measured from (a) AlN/Si, (b) AlN/Mo, and (c) AlN/W.

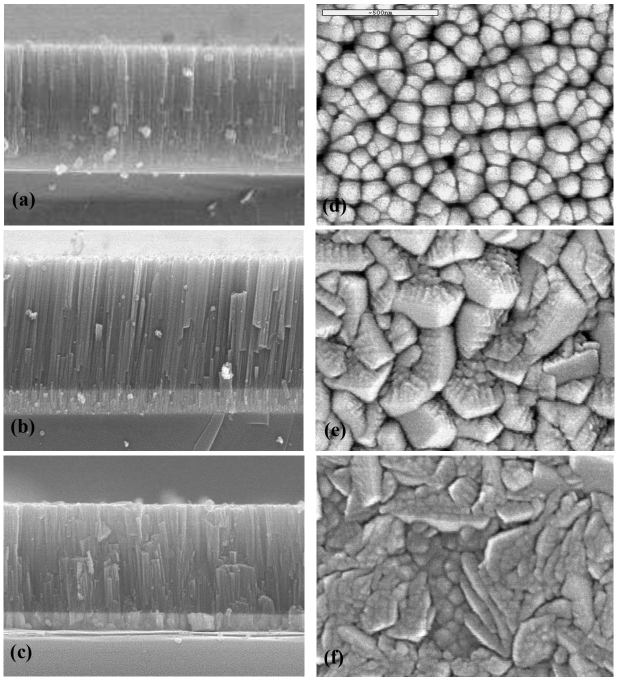

Figure 2. SEM image measured from AlN/Si ((a), (d)), AlN/Mo ((b), (e)), and AlN/W ((c), (f))

In addition, (002)-orientation and surface morphologies of the AlN films deposited on various substrates were investigated using SEM, as shown in Fig. 2(a) ~ (f). It can be seen that the AlN films (Fig. 2(a), (d)) directly deposited on Si (111) exhibited better c-axis growth behavior and possessed more uniform grains and smoother surface than that deposited on Mo (Fig. 2(b), (e)) and W (Fig. 2(c), (e)) films, respectively. Besides, it was founded that the AlN films deposited on Mo have superior (002)-orientation and surface morphologies, compared to that deposited on W.

As can be seen from Fig.1 and Fig. 2, the Mo film as a bottom electrode, which affects the properties of piezoelectric materials (AlN) in a FBAR structure, can be considered as a suitable material.

B. Effects of deposition conditions on AlN properties

In this research, the effects of process variables on the (002) preferred orientation and crystal quality of AlN films deposited on the Mo layer have been systematically investigated. The related results are presented in Fig. 3(a) ~ (c) which show the dependence of ω-FWHM and TC values of AlN/Mo films on the deposition variables.

In more detail (see Fig. 3(a)), the ω-FWHM of AlN was found to monotonically decrease with RF power. It has been reported that in the AlN structure the bond energy of Al-N bond in the direction of c-axis is relatively smaller than that of other bonds and is easy to break, so that a large energy is required for sputtering particles to be deposited in the direction of the c-axis [7]. This may be the reason why the increasing RF power resulted in better crystal quality of AlN films. However, as the RF power increased, the TC values of the AlN decreased. Also, as the N_2/Ar ratio increased (Fig. 3 (b)), the ω-FWHM increased and TC values decrease. Finally, the ω-FWHM increased with working pressure (Fig. 3(c)). This is attributed to the decrease of the mean free path of Al atoms which participate in the AlN deposition. The mean free path of Al atoms sputtered from the target may depend on the collision probability which may increase at high pressure, hence leading to the loss of kinetic energy of Al atoms [8-10].

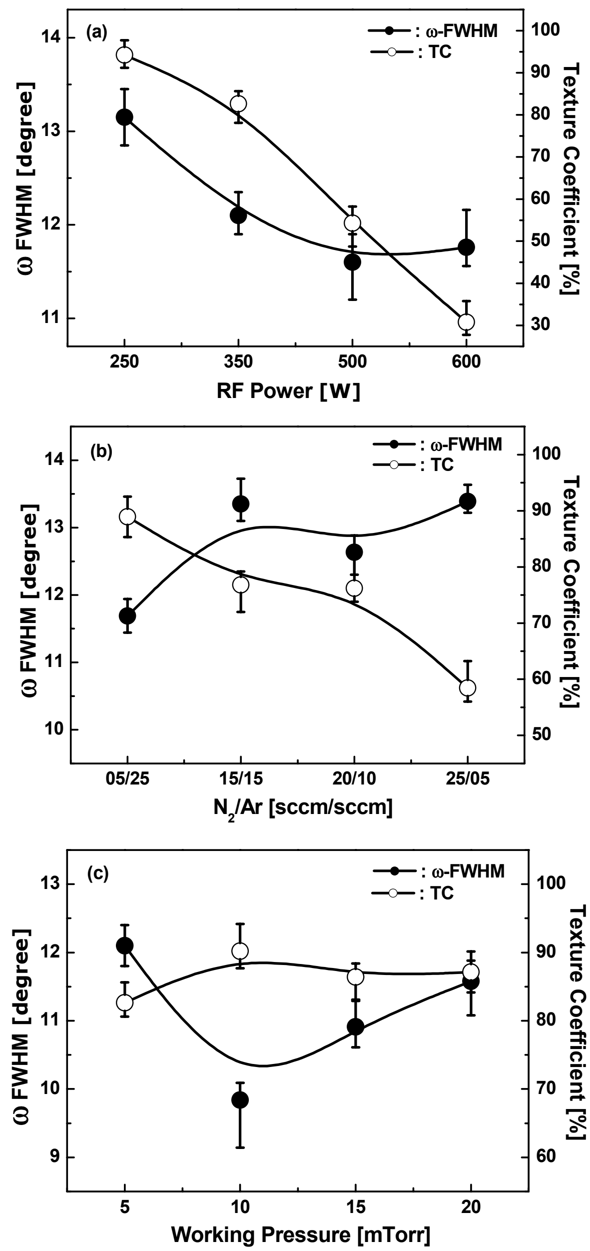

Figure 3. The estimated FWHM and (002)-TC values of AlN films as a function of (a) RF power, (b) N_2/Ar ratio, and (c) working pressure.

C. FBAR characteristics in terms of AlN properties

Fig. 4 shows the frequency response (S_{11}) of FBARs as a function of ω-FWHM, TC, and RMS surface roughness (σ_{rms}). As shown in the figure, the higher the TC values in AlN films, the larger return loss of FBARs resulted. In addition, a shift of resonant frequency to lower frequency was observed. This may be attributed to the increase of thickness of AlN film [11].

To examine relationship between properties of AlN film and characteristics of FBARs, electromechanical constant and return loss have been measured for all fabricated FBARs. As shown Fig. 5(a) ~ (c), the return loss increases with increasing (002)-TC value. The return loss was relatively high at the large RMS surface roughness of the AlN film. However, varying the ω-FWHM value, the variation of return loss was relatively small. It should be noted that the return loss of ω-FBARs strongly depended on the texture coefficient and surface roughness of AlN films.

For the electromechanical constant of FBARs, it increased as the ω-FWHM value of AlN film increased (Fig. 5(d)). High electromechanical constant was also observed at relatively large RMS roughness of the AlN film (Fig. 5(f)). It is noticed that the electromechanical coefficient of FBARs strongly depended on the ω-FWHM value and RMS surface roughness of the AlN films. This indicates that the characteristics of the FBAR devices may be strongly affected by material properties of the AlN films, as shown in the above results.

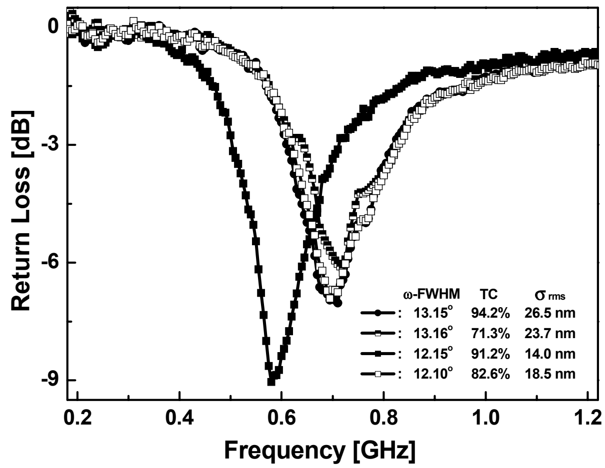

Figure. 4 Frequency response of FABRs as a function of FWHM, (002)-TC, and RMS surface roughness

D. BVD parameter in terms of AlN properties

To establish a theoretical relationship for formulating the impedance of FBARs as a function of material properties, the relationship between the motional resistance (R_m) and the material properties of AlN films was investigated by simulating a BVD model. Fig. 6(a) ~ (c) shows the BVD model parameter (R_m) as a function of AlN properties. As (002)-TC and ω-FWHM value increased, the motional resistance increased. The smoother the RMS surface roughness,

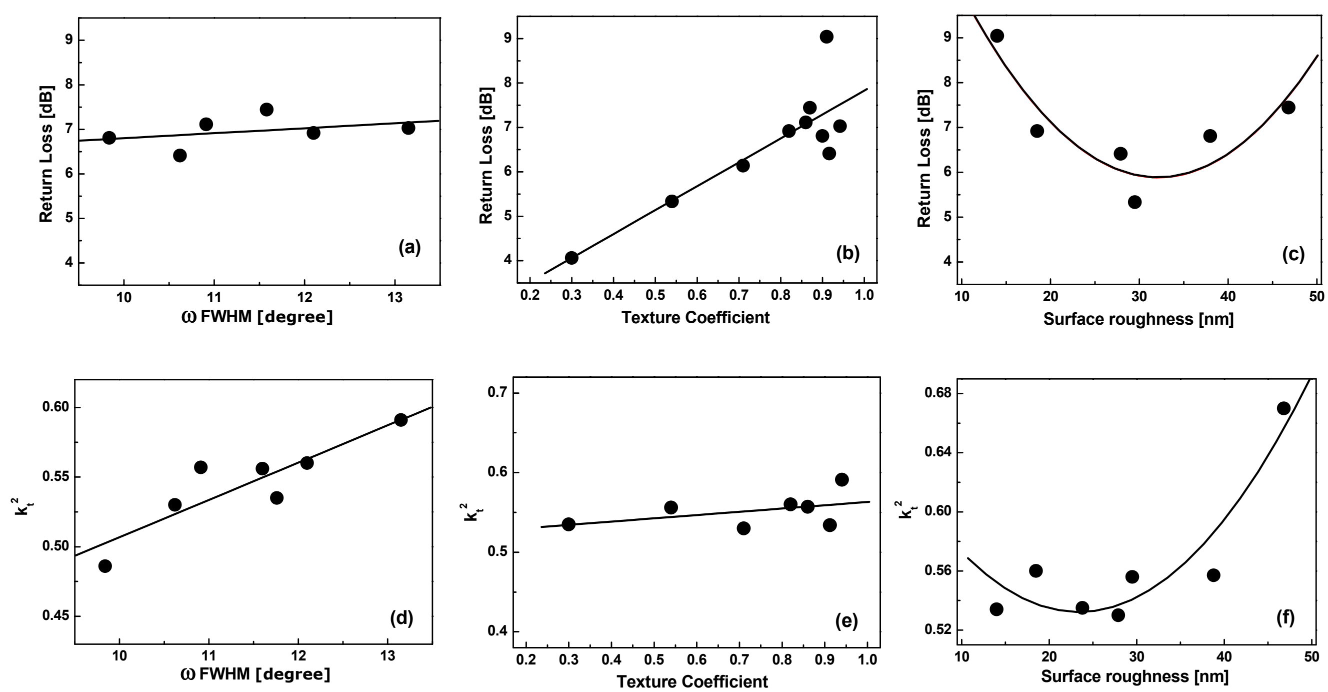

Figure 5. The characteristics such as RL ((a) ~ (c)) and k_t^2 ((d) ~ (f)) of FBARs as a function of material properties of AlN films

the higher the motional resistance occurred. It should be noted that the dependence of motion resistance on the properties of AlN films have almost tracked that of the return loss. It was also expected that the motional resistance was directly extracted by establishing the relationship between the material properties of the AlN films without measuring the electrical properties (i.e, frequency response, Q factor) of FBARs.

Fig. 7 shows the frequency response characteristics of the FBARs obtained from measurement and the proposed relationship. It is noted that the experimentally measured result was in good agreement with that obtained from the proposed relationship.

Fig. 8(a) and (b) show the frequency response characteristics of FBARs obtained from both the BVD model and the proposed relationship. The BVD model was simulated by using the experimentally measured motional resistance values. In the proposed relationship, the three fitting parameters, such as ω-FWHM, (002)-TC, and RMS surface roughness, are used to obtain the frequency response curves. The parameters values for various FBAR devices (device ID: (i) ~ (v)) are listed in Table 2. By comparing Fig. 8(a) to Fig. 8(b), it should be noted that the BVD model result was in good agreement with that obtained from the proposed relationship.

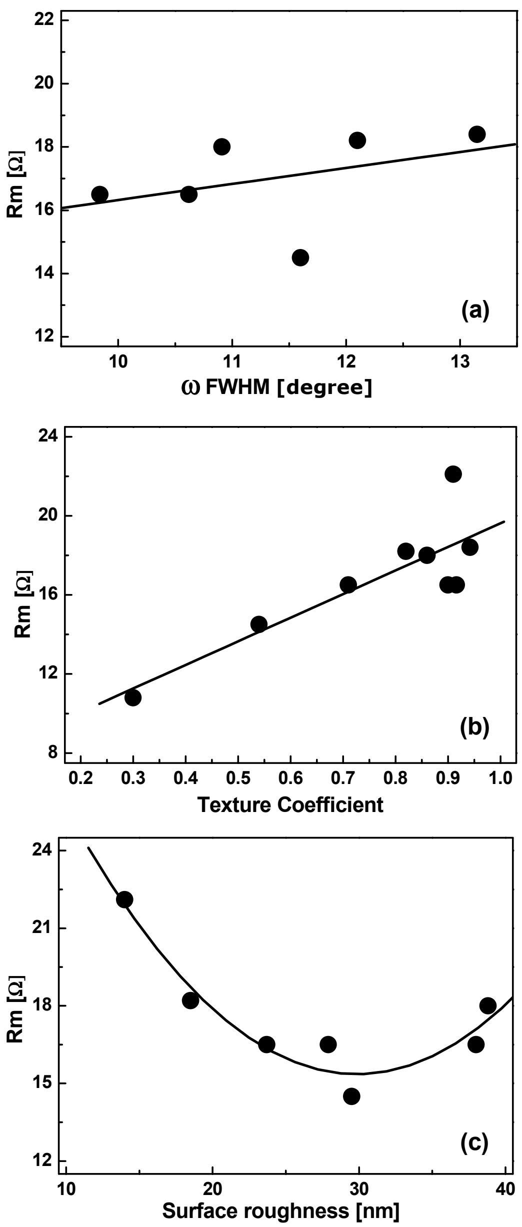

Figure 6. BVD model parameter (R_m) as a function of material properties of AlN films

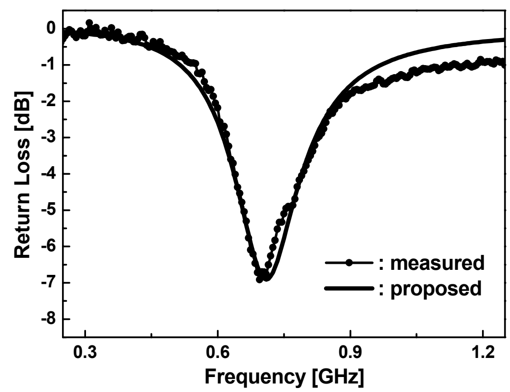

Figure 7. Frequency response characteristics of FBARs (measurement vs. proposed relationship)

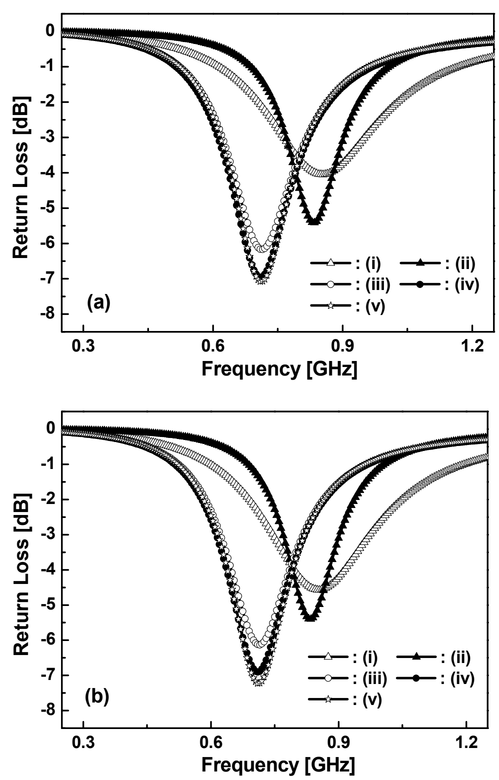

Figure 8. Frequency response characteristics of FBARs obtained by using (a) BVD model and (b) proposed relationship.

Table 2. Fitting parameters used in the proposed relationship (Fig. 8(b))

Device ID	(i)	(ii)	(iii)	(iv)	(v)
FWHM [^{o}]	11.7	11.6	13.1	12.1	13.1
TC [%]	30.7	54.2	71.3	82.6	86.4
σ_{rms} [nm]	23.8	29.5	23.7	18.5	38.8

IV. CONCLUSION

In this paper, we have investigated the effects of deposition conditions on the structural properties of AlN films, such as ω-FWHM, (002)-TC, and RMS surface roughness. The measurements of return loss and electromechanical constant of FBARs confirm that the crystal quality of AlN films strongly affects the characteristics of the FBARs. In addition, the dependence of motional resistance (R_m) on the properties of AlN films has closely tracked the variation of return loss. In addition, a theoretical relationship between the motional resistance and the AlN properties (ω-FWHM, (002)-TC, and RMS surface roughness) has been established. The results confirm that the frequency response of FBARs obtained from the proposed relationship is in good agreement with the experimentally measured data.

ACKNOWLEDGMENTS

This work carried out using the facilities of center for Electronic Materials and Components (EM&C) in Hanyang University

REFERENCES

[1] K.M. Lakin, "Thin Film Resonators and Filters", *IEEE Ultrasonics Symp*., pp. 895-906, 1999.

[2] R.S. Naik, J.J. Lutsky, and R. Reif, "Measurements of the Bulk, C-Axis Electromechanical Coupling Constant as a Function of AlN Film Quality", *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.* Vol. 47, pp. 292-296, 2000.

[3] R.A. Naik, R. Reif, J. J. Lutsky, and C. G. Sodini, "Low-Temperature Deposition of Highly Textured Aluminum Nitride by Direct Current Magnetron Sputtering for Applications in Thin-Film Resonators", *J. Electrochem. Soc.*, 146, pp. 691-696, 1999.

[4] J.D. Larson III, P.D. Bradley, S. Wartenberg, and R.C. Ruby, "Modified Butterworth-Van Dyke Circuit for FBAR Resonators and Automated Measurement System", *IEEE Ultrasonics Symp.*, pp. 863-868, 2000.

[5] K.M. Lakin, K.T. McCarron, J. Belsick, and J.F. McDonald, "Thin Film Bulk Acoustic Wave Resonator and Filter Technology", *IEEE*, pp. 89-92, 2001.

[6] M. Akiyama, T. Harada, C.N. Xu, K. Nonaka, and T. Watanabe, "Preparation of highly oriented AlN thin films on glass substrates by helicon plasma sputtering and design of experiments", *Thin Solid Films* 350, pp. 85-90, 1999.

[7] X.H. Xu, H.S. Wu, C.J. Zhang, and Z.H. Jin, "Morphological properties of AlN piezoelectric thin films deposited by DC reactive magnetron sputtering", *Thin Solid Films* 388, pp. 62-67, 2001.

[8] T. Shibata, K. Asai, Y. Nakamura, M. Tanaka, K. Kaigawa, J. Shibata, and H. Sakai, "AlN epitaxial growth on off-angle R-plane sapphire substrates by MOCVD", *J. Crystal Growth* 229, pp. 63-68, 2001.

[9] J.H. Lee, W.M. Kim, T.S. Lee, M.K. Chung, B.K. Cheong, and S.G.. Kim, "Mechanical and adhesion properties of Al/AlN multilayered thin films", *Surf. Coat. Technol.* 133-134, pp. 220-226, 2000.

[10] S. Uchiyama, Y. Ishigami, M. Ohta, M. Niigaki, H. Kan, Y. Nakanishi, and T. Yamaguchi, "Growth of AlN films by magnetron sputtering", *J. Crystal Growth* 189/190, pp. 448-451, 1998.

[11] P. Osbond, C.M Beck, C.J. Brierley, M.R. Cox, S.P. Marsh, and N.M. Shorrocks, "The Influence of ZnO and Electrode Thickness on the performance of Thin Film Bulk Acoustic Wave Resonators", *IEEE Ultrasonics Symp.*, pp. 911-914, 1999.