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Frequency responses of an AlN/IDT/Si surface acoustic wave device based on AlN thin films with different grain sizes

Soo Ho Kim, Kwang Hoon Lee, Dong-Joo Kim[a] and Young Soo Yoon*

Department of Advanced Technology Fusion, Konkuk University, 1 Hwayang-dong, Gwangjin-gu, Seoul 143-701, Korea
[a]Materials Research and Education Center, Dept. of Mechanical Engineering, Auburn University, 201 Ross Hall, AL 36849-5341, USA

Frequency responses of AlN/IDT/Si surface acoustic wave structures with single and double interdigital transducer (IDT) patterns were characterized to investigate the grain-size effects of AlN piezoelectric thin films deposited by a sputtering method. In order to control grain size of films, r.f. sputtering powers were varied at 200 and 300 W. The as-deposited AlN film prepared at 300 W had a larger grain size than the film deposited at 200 W, but the grain shape of the as-deposited films was almost identical irrespective of r.f. power, which indicates larger grain-boundary area for the as-deposited film at 200 W. The as-deposited films prepared at 300 W and 200 W showed full width half at maximum values of 3.54° and 4.41° at the X-ray peak of 2θ = 36°, respectively. In the frequency response measurements, better frequency properties were obtained in the as-deposited AlN film with an r.f. power of 300 W. For example, the electromechanical coupling factor of the as-deposited AlN film at 300 W was 0.13%, while that of the as-deposited AlN film at 200 W was 0.10%. From a frequency response analysis, the grain size was found to affect the frequency response strongly. These results indicate that AlN thin film promises high potential for a high frequency device if a highly-textured AlN film with large grain size can be deposited.

Key words: Piezoelectric thin film, Sputtering, High frequency, Grain size.

Introduction

Recently, high frequency-based electronic devices, such as surface acoustic wave (SAW) and bulk acoustic wave (BAW), have been intensively studied since these devices are the core components for mobile communication applications [1-4]. In order to develop high performance devices, piezoelectric ceramics have been rigorously investigated for many years. Typical piezoelectric ceramics for such investigation include ZnO, $LiNbO_3$ and $LiTaO_3$. For example, SAW devices used for the application of hand-carried communication systems based on code division multiple access (CDMA) such as cellular phones are developed by constructing components using bulk-type single crystalline piezoelectric ceramics.

These bulk type single crystalline ceramics, however, have limitations such as size reduction, high cost and high power consumption. These problems can be solved when thin films piezoelectric ceramics are synthesized such that a SAW device requires low levels of power and can be fabricated in an economic and easy way. These benefits can be realized not only when we deposit the highly-oriented crystalline structure of these piezoelectric materials, but also when we use photolithography to achieve complex high resolution interdigital transducers (IDT) that results in miniature and high performance devices.

In general, vast amounts of information can be delivered when communicating electronic devices use high frequency range above a gigahertz. Unfortunately, conventional piezoelectric ceramics as mentioned above do not match this frequency range. A Wurtzite hexagonally structured AlN consisting of ionic and covalent bonding characteristics can be an emerging candidate for the gigahertz level due to its fast wave propagation velocity, high piezoelectric constant, and high electrical resistivity [5-10]. In addition, AlN can be easily deposited in a thin film form for the integration of SAW devices. Above all, AlN thin films integrated onto a Si semiconductor substrate can realizee high performance, high frequency devices due to possible deposition at a relatively low temperature compatible with Si processes and the similar thermal expansion coefficient between the bulk AlN and Si. Fabrication of AlN thin films directly on Si is also very advantageous and crucial since Si-based processes allow easy and inexpensive integration [11-13]. However, few studies have been done on AlN thin films deposited on Si for SAW applications, to our knowledge, even though purely c-axis oriented AlN thin films on $LiNbO_3$, quartz and diamond-like carbon have been reported [14-16]. As-grown AlN thin films grown on a diamond substrate or a (0001) Al_2O_3 substrate have been considered as a possibility for high frequency applications due to the large mismatch between Si and AlN.

*Corresponding author:
Tel : +82-2-2049-6042
Fax: +82-2-452-5558
E-mail: ysyoon@konkuk.ac.kr

The sputtering technique has been employed due to possible deposition of AlN thin films with sufficient quality for high frequency-based devices. For example, Clements and coworkers [12] have used r.f. reactive sputtering to grow crystalline AlN thin films on (100) and (111) Si substrates to fabricate high-frequency SAW devices. They reported the influence of the process parameters on the structural properties of the as-deposited AlN thin films. However, the relationship between the structural properties of the as-deposited AlN thin films and the frequency response of IDTs with AlN thin films has not yet been adequately investigated or reported. In particular, no reports have clearly demonstrated the possibility of high-frequency devices based on AlN thin films on Si substrates.

In this study we focused our attention on the deposition of AlN thin films on (100) Si substrates by r.f. reactive sputtering at room temperature and on the relationship between the structural properties of AlN thin films and the frequency response of IDTs with double electrodes.

Experiments

We used 4 inch (100 mm) Al (99.999%) metal discs as a sputter target and a plasma mixture of Ar and N_2 (1:2) as the sputtering gases both with a purity of 99.999%. The (100) Si substrates were degreased in warm acetone and trichloroethylene (TCE) three times, rinsed in deionized water with a resistivity of above several 10^8 ohm·cm thoroughly, etched in a mixture of H_2SO_4, H_2O_2 and H_2O (4:1:1) at 40 °C for 10 minute, and rinsed in TCE again. After the Si substrates were evacuated to 0.00027 Pa, the depositions were performed at room temperature. Prior to AlN growth, the Al target was cleaned to remove surface contaminations by Ar^+ sputtering ions only. The deposition of AlN thin films were carried out on the 4 inch (100 mm) (100) Si substrates using a horizontal on-axis type r.f. (13.56 MHz) reactive sputter with two different powers of 200 and 300 W. The working pressure was 0.67 Pa.

Cross-sectional scanning electron microscopy (SEM) and α-step were utilized to confirm the thickness of AlN films with 1 mm thickness. Wide angle XRD ($CuK_\alpha = 1.5406$ Å) measurements were taken to measure the crystallinity of the as-deposited AlN thin films with a deposition area of 1×1 cm^2. The frequency response measurements of as-deposited AlN films were performed using a Caltec Intermediate Form (CIF) program. We designed the IDT patterns with an input of 30 single electrodes and an output of 15 double electrodes. The IDT were patterned after deposition of a metallic Al thin film on the (100) Si substrate using a lift-off method based on a photolithography process. The specifications of the as- fabricated IDT patterns and the fabrication specifications are shown in Table 1, a and the final sample structure is AlN/Al-IDT/Si. In order to minimize any external signal noise, all samples for frequency measurements were encased in an Al metal box.

Table 1. Specifications for fabricating the IDT

Parameters	Specification	
	Single electrode	Double electrode
Electrode width	2 μm	2 μm
Electrode space	2 μm	2 μm
Electrode aperture	400 μm	800 μm
Wavelength	8 μm	16 μm
Propagation length	160 μm	320 μm
Number of electrode pair	60	30

Results and Discussion

The wide XRD patterns for AlN thin films deposited at different r.f. powers are shown in Fig. 1. The AlN films show an (002) AlN peak at 2θ=36° regardless of the r.f. power, which indicates that the c-axis of AlN thin film is perpendicular to the surface of the Si substrate. These XRD results can signify that both as-deposited AlN films have a strong c-axis-preferred orientation even though the applied r.f. power during the depositing process was different each other. In addition, both films do not show other diffraction peaks than AlN. There exists, however, a difference of XRD peak intensity. The wide XRD patterns of AlN film deposited at 200 W exhibit a lower intensity of the (002) peak, which is attributed to a smaller grain size than that of AlN film deposited at 300 W as shown in the SEM images (Fig. 2). In addition, the SEM surface micrographs present that as-deposited AlN films show typical polycrystalline surface structure with strong (002) preferred

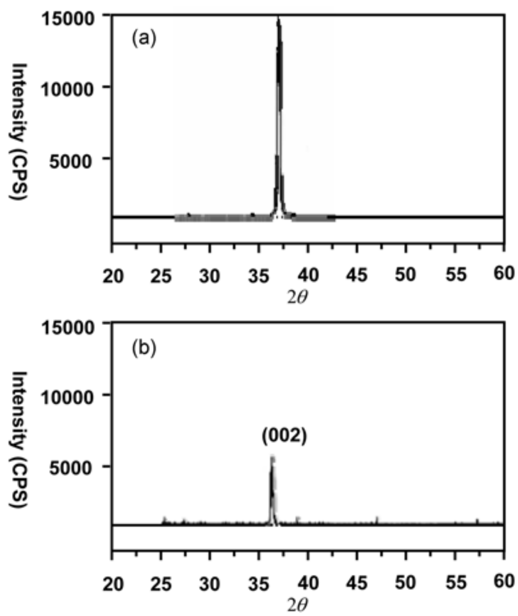

Fig. 1. Wide XRD patterns for the as-deposited AlN films.

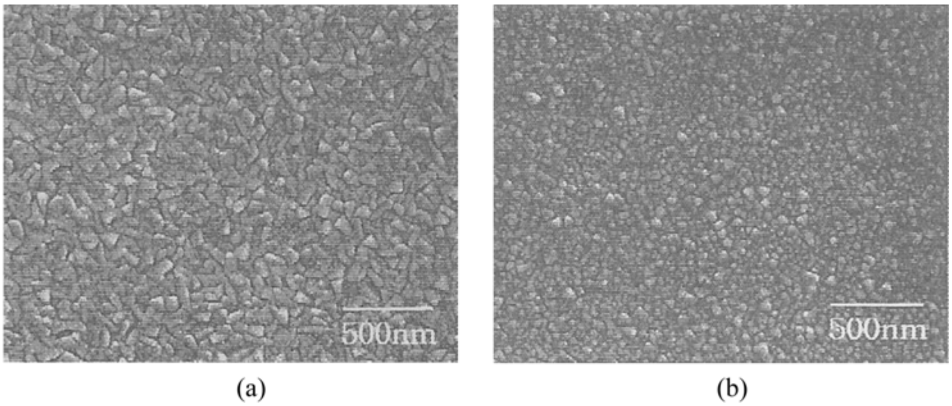

Fig. 2. SEM Surface images of the as-deposited AlN films deposited at (a) 300 W and (b) 200 W.

orientation which was observed in the XRD patterns. This is likely that both as-deposited films at 200 W and 300 W contain (002) textured poly crystalline grains with a misalignment of the a and b axes. When compared with the surface SEM images of as-deposited AlN films, the grain shapes are similar to each other while the grain size of AlN film at 300 W is almost twice the size of the film deposited at 200 W. Therefore, we can speculate larger grain-boundary area of AlN film at 200 W than that of AlN film at 300 W.

The full width half at maximum (FWHM) values of the (002) peak were compared in order to investigate the structural characteristics in more detail. The FWHM was 3.54° for as-deposited AlN film at 300 W while the value increased to 4.41 at 200 W. Although the AlN films deposited at both 200 W and 300 W exhibited only a (002) preferred orientation, the FWHM of the film deposited at 300 W is smaller than that at 200 W. This broadening FWHM value can be presumed to represent different crystallinity between the films at 300 W and 200 W, and this feature shown in the FWHM of (002) peaks can be due to a different grain size and/or the residual strain level. The grain size and the residual strain induced by interfaces and/or grain-boundaries can contribute to the broadening of a XRD peak, which can be expressed by the following equation: [17]

$$\beta = k\lambda/(d\cos\theta) + \varepsilon\tan\theta$$

where, β is the corrected FWHM, θ is the diffraction angle, d is the grain size, ε is the strain and λ is the wavelength of the X-rays. k is a constant with a value of 0.94 if the grain size of the as-deposited film is uniform. Even though as-deposited AlN films show different peak intensities of the (002) maxima, both films have a polycrystalline textured structure. Therefore, a significant level of difference in residual strain might not be found between both AlN films, that is, no strain was induced by a lattice constant difference between the substrate and the as-deposited AlN film. Hence, the β is proportional to the grain size since the values of ε are almost the same for both films. Since the θ values are almost same for both AlN films, the above equation, finally, can be thought as follows :

$$\beta \propto k\lambda/(d\cos\theta) \propto k\lambda/d$$

This relationship can explain that as-deposited AlN film at 300 W shows larger grain size than the film deposited at 200 W, which can be confirmed by the surface SEM images as shown in Fig. 2.

We can presumably interpret the increase of the grain size by assuming that a high sputtering power (300 W) can induce high kinetic energy of the sputtered particles from the target. This process increases the mobility of the as-sputtered particles when these arrived at the substrate surface. Finally, the kinetic energy of the as-deposited particles on the substrate had sufficient energy to efficiently migrate to the surface for the formation of a relatively larger grain.

Table 2 details the frequency response characteristics observed at room temperature for AlN thin films with the IDT electrode pattern shown in Table 1. The parameters of the center frequency and band width are not very different for AlN films deposited at different sputtering powers. However, the electromechanical coupling factor, propagation velocity and the insertion loss show larger differences above 10%. In general, the frequency response characteristics depend on the properties of the thin film and the geometry of the device. In this study, the same device geometry was used regardless of the sputtering conditions. Therefore, the differences in fre-

Table 2. Characteristics of the frequency response

Deposition pressure	Center frequency	Propagation velocity	Electromechanical coupling factor	Insertion loss	Band width
300 W	400 MHz	5200 m/s	0.13%	28 dB	12.5 MHz
200 W	396 MHz	4600 m/s	0.10%	33 dB	12.9 MHz

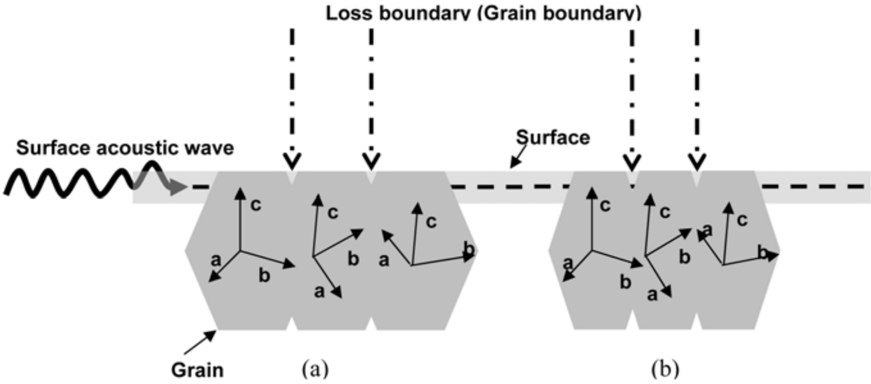

Fig. 3. Schematic diagram of the wave propagation profile on the surfaces of the AlN films deposited at (a) 300 W and (b) 200 W.

quency response originate from the difference in the grain size.

By comparing Fig. 3, which shows a schematic diagram of the wave propagation profile on the surfaces of the as-deposited AlN film and Table 2, we can deduce that the size difference of the grains with the same textural property strongly influences the important device properties such as the electromechanical coupling factor, propagation velocity and the insertion loss. However, other properties are not so strongly dependent on the grain size. These results reveal that the grain boundary density should be reduced to improve the high frequency characteristics such as the electromechanical coupling factor, propagation velocity and the insertion loss. Even though the values of the electromechanical coupling factor and the insertion loss of as-deposited AlN thin film at 300 W are inadequate for real applications, AlN thin films deposited on an Si substrate with the IDT at room temperature manifestly show the great potential for high frequency application based on a piezoelectric thin film.

Conclusions

In conclusion, AlN thin films with a highly (002) textured orientation and different grain sizes on (100) Si substrates were deposited using r.f. reactive magnetron sputtering at room temperature in order to investigate the feasibility for a high frequency device based on a piezoelectric thin film. With respect to the wide XRD pattern, both AlN films deposited at 200 W and 300 W show (002) peaks and no other crystalline peaks; in contrast, the intensity of the (002) peak of the film deposited at 300 W is larger than that of the film at 200 W. We also observed an XRD FWHM value of 3.54° in the film deposited at 300 W, while the as-deposited film at 200 W had 4.41°. Based on single and double IDT electrode patterns on the Si substrate, many frequency response characteristics such as electromechanical coupling factor, propagation velocity and the insertion loss strongly depend on the grain size. In contrast, the center frequency and the band width do not show strong dependence of these properties on the grain size. Our results clearly reveal that AlN thin films deposited at room temperature can offer possibilities for fabricating piezoelectric-based high frequency electronic devices, if very highly textured AlN films with large grain size on Si substrates could be deposited.

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