GROWTH OF HIGHLY C-AXIS ORIENTED ALN FILMS ON 3C-SiC/Si SUBSTRATE

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ABSTRACT

For the first time, highly *c*-axis oriented heteroepitaxial AlN thin films have been successfully grown on epitaxial 3C-SiC films on Si (100) substrates. The AlN films deposited by the AC reactive magnetron sputtering at temperatures of approximately 300–450 °C were characterized using the scanning electron microscope (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), and transmission electron microscopy (TEM). X-ray diffraction rocking curve of 1- μ m-thick AlN film exhibits a full width at half maximum (FWHM) value of 1.73° on the 3C-SiC/Si substrate which correlates to the excellent crystal alignment of the AlN film. Finally, two-port surface acoustic wave (SAW) devices were fabricated on the AlN/3C-SiC/Si composite structure, and the expected Rayleigh mode of the SAW device exhibits a high acoustic velocity of 5,200 m/s, demonstrating the potential for high frequency applications. The AlN/3C-SiC/Si composite structure developed in this work has potential for realizing radio frequency (RF) MEMS resonators and filters as well as piezoelectric MEMS sensors and actuators for operation in harsh environments.

INTRODUCTION

Recently, silicon carbide (SiC) has been investigated as a platform material to create electronics, sensors, and actuators for harsh environments (high temperature, high shock, and chemically corrosive conditions) due to the thermal, mechanical, and electrical stability of this material [1]. Although SiC has over 200 different crystal symmetries, the cubic (3C-SiC) and the hexagonal (4H-SiC and 6H-SiC) polytypes are most commonly synthesized. Among these polytypes, chemical vapor deposition (CVD) of in-situ doped polycrystalline 3C-SiC deposited on Si substrates has been achieved by many academic research groups [1, 2]. An industrial group also has commercialized epitaxial 3C-SiC thin films deposited on Si substrates [3]. The advancement of SiC manufacturing technology enabled the fabrication of electrostatic SiC comb-drive actuators and sensors [4] using low-pressure chemical vapor deposition (LPCVD) polycrystalline 3C-SiC films. Electrostatic resonators made from polycrystalline 3C-SiC have been developed for RF MEMS applications [5, 6] and show promise for these applications due to the high acoustic velocity of 13,000 m/s and low losses [7].

Piezoelectric actuation method is a viable alternative to the electrostatic actuation method frequently used for MEMS devices. Although SiC exhibits piezoelectric properties, its low piezoelectric coefficient makes it unsuitable for device designs [8]. To overcome this limitation, the deposition of piezoelectric thin films onto 3C-SiC could be an alternative method to drive SiC-based MEMS devices utilizing the piezoelectric effect. Aluminum nitride (AlN) has been widely applied to RF MEMS devices because of its relatively high piezoelectric coefficient, CMOS compatibility, and high acoustic velocity of 12,000 m/s [8]. In general, AlN and SiC exhibit the well-matched thermal expansion coefficient and low lattice mismatch [9]. AlN can maintain its piezoelectric properties at high temperatures as well [10, 11]. Therefore, coupling AlN and 3C-SiC to create a composite structure could be advantageous for RF MEMS and harsh environment applications.

Several research groups have investigated and successfully deposited ZnO or AlN films on hexagonal SiC substrates [7, 12, 13]. However, the hexagonal SiC polytypes are unsuitable for MEMS devices because it is difficult to grow hexagonal SiC films on silicon wafers. In addition, there are a few reports detailing the deposition of AlN thin films on 3C-SiC substrates. For example, Tanaka *et al.* deposited AlN (100) thin films on 3C-SiC (001) using low-pressure metal-organic chemical vapor deposition (LP-MOCVD) method [14]. Chung *et al.* used a layer of polycrystalline 3C-SiC film as the buffer layer for AlN (002) deposition on Si (100) substrates using the AC magnetron reactive sputtering because the polycrystalline 3C-SiC buffer layer and AlN film have only 1% lattice mismatch and 7% difference in the thermal expansion coefficient [15].

In this study, the deposition of highly oriented AlN (002) films on 3C-SiC(100)/Si(100) substrates using AC reactive magnetron sputtering is developed and experimentally investigated. Although the heteroepitaxial AlN film (002) and the epitaxial 3C-SiC (100) film have a larger lattice mismatch of 28.6%, this issue could be overcome by a two-step deposition process. After AlN deposition on the SiC/Si substrate, two-port SAW devices were fabricated on the AlN/3C-SiC/Si composite structure to confirm that the AlN thin film has strong piezoelectric response. These results create a basis for the development of piezoelectric AlN/3C-SiC-based MEMS devices for frequency control and sensing applications in harsh environments.

EXPERIMENTS

For this research, wafers with 2.3- μ m-thick epitaxial 3C-SiC (100) films grown on Si (100) substrates were purchased from the NOVASiC Inc. [3]. AlN thin films with different thicknesses in the range of 1 μ m to 3 μ m were deposited on 3C-SiC/Si substrates by AC (40 kHz) powered S-Gun magnetron. A unique feature of the S-Gun is its coaxial dual target arrangement that enables arc-less operation in poison mode with capability for independent control of the film crystal orientation, stress, and uniformity [16].

Prior to AlN thin film deposition, the surface of the 3C-SiC/Si substrate was treated in a separate etching module by low energy (150–200 eV) Ar ions from capacitively coupled RF (13.56 MHz) plasma. In order to diminish the lattice mismatch between the AlN film and the 3C-SiC substrate, a two-step sputter deposition process was employed in this study to create better conditions for nucleation of AlN grains at the beginning of the film condensation. For this purpose, a first 50-nm-thick AlN film was deposited with high nitrogen concentration in argon and nitrogen gas mixture. The initial grains served as the seeds for the growth of higher quality columnar grains with the increase of AlN film thickness. This seed layer also enabled reducing the negative effect of lattice mismatch between the AlN thin film and the 3C-SiC substrate.

The seed layer deposition processes were performed at the ambient temperature (around 300 °C) and the elevated temperature (around 450 °C) using an external infrared heater. S-Gun magnetron was powered with an AC power of 3 kW during the seed layer deposition and 5.5 kW during the deposition of the remaining AlN film, providing a deposition rate of approximately 66 nm/min.

Figure 1: Cross-sectional SEM image of 1- μ m-thick AlN (002) film on the 3C-SiC(100)/Si(100) layered structure.

Figure 2: AFM images of 3C-SiC (100) and AlN (002) films.

Figure 3: XRD spectrum of the AlN(002)/3C-SiC(100)/Si(100) layered structure where AlN is 1 μ m and 3C-SiC is 2.3 μ m.

RESULTS AND DISCUSSIONS

A. Heteroepitaxial AlN (002) films on 3C-SiC(100)/Si(100)

Figure 1 shows the cross-sectional SEM image of the AlN(002)/3C-SiC(100)/Si(100) composite structure where the AlN and 3C-SiC film thicknesses are 1 μ m and 2.3 μ m, respectively. The void defects with pyramidal shape at the 3C-SiC/Si interface are due

Figure 4: Rocking curve of 1- μ m-thick AlN (002) film.

to silicon outdiffusion. The interface between AlN and 3C-SiC is smooth and no delamination is observed. The AlN thin film exhibits numerous columnar grains which are perpendicular to the surface of the 3C-SiC/Si substrate. The surface morphology of the 3C-SiC and AlN films is shown in Figure 2. According to the AFM data, the root mean square (RMS) roughness of the 3C-SiC and AlN films are 5.9 nm and 2.9 nm, respectively. The preservation of the 3C-SiC grain boundary and the RMS roughness on the AlN surface implies that the nucleation is two-dimensional growth.

The crystalline structure was determined by XRD as shown in Figure 3 where the diffraction peaks correspond to a hexagonal wurtzite-type AlN (002) film, a cubic zinc-blende-type SiC (100) film, and a Si (100) substrate, respectively. The presence of (002) and (004) AlN reflections gives the indication of a highly *c*-axis oriented AlN film that has been grown on the 3C-SiC(100)/Si(100) substrate. As shown in Figure 4, the rocking curve FWHM of the 1- μ m-thick AlN film is 1.73° which implies the highly oriented AlN film and good piezoelectric property.

Besides directly depositing AlN thin films onto the 3C-SiC/Si substrate, several different surface pretreatments of the substrate and deposition at the ambient or elevated temperatures were employed to investigate their effects on AlN film crystallinity as shown in Figure 5 and Table 1. The rocking curve FWHM of the AlN film can be improved from 2.61° to 2.29° when the deposition temperature in the first step deposition (i.e. seed layer deposition) was increased from ambient temperature to elevated temperature.

In addition to the sputter conditions, the degree of *c*-axis texturing of the reactively sputtered AlN film is closely related to the substrate texture and the surface roughness. Therefore, the pretreatment of the 3C-SiC/Si substrate can significantly influence the AlN film orientation. It is well-known that pre-deposition RF plasma etching can improve the film nucleation and coalescence processes due to removal of impurities. Furthermore, the RF plasma etching can decrease the surface roughness of the substrate and hence improve the AlN crystal alignment. As depicted in Figure 5, a relatively longer RF plasma etching duration of 600 s is required to achieve the better crystallinity of AlN thin films on 3C-SiC substrates. For comparison, the RF plasma etching duration of 180 s is enough to get highly *c*-axis oriented AlN thin films on silicon wafers under the same sputter conditions. This phenomenon might be due to the higher atomic binding energy and the lower sputtering yield of SiC. The sputtering yield ratio for silicon carbide to silicon is approximately 0.5 [8].

Figure 5: The plot of measured FWHM of AlN under different pre-deposition conditions versus AlN film thicknesses.

Figure 6: The cross-sectional bright field TEM image of the interface between AlN (002) and 3C-SiC (100).

Figure 7: Electron diffraction patterns of 1-μm-thick AlN film grown on the 3C-SiC(100)/Si(100) substrate along the [110] zone axis of the AlN film.

Table 1: Pre-deposition treatment conditions for different AlN film thicknesses and their related FWHM values.

Duration of RF plasma etching	Seed layer deposition temp.	AlN thickness	AlN FWHM
180 s	ambient	1 μm	2.61°
180 s	elevated	1 μm	2.29°
360 s	elevated	1 μm	1.89°
600 s	elevated	1 μm	1.73°
600 s	elevated	1.5 μm	1.62°
600 s	elevated	2 μm	1.51°
600 s	elevated	2.5 μm	1.36°
600 s	elevated	3 μm	1.31°

The X-ray rocking curve measurements have shown that the crystal orientation of AlN films on 3C-SiC/Si substrates can be improved with increasing the film thickness due to development of more thorough columnar grains. The best texture with a FWHM value of 1.31° was achieved in the 3-μm-thick AlN film, which was deposited using two-step process: the first seed layer of 50-nm-thick AlN film was deposited at elevated temperature and the following well-textured AlN film was deposited at ambient conditions during the second step deposition process. Actually, a permanent heating at elevated temperature during the entire deposition process did not remarkably improve the crystal orientation, indicating that higher adatom mobility is required mostly at the nucleation stage which ensures the grain formation with less structural defects and releases the relatively large lattice mismatch of AlN and 3C-SiC as well. For comparison, 1-μm-thick AlN films deposited at ambient conditions and using the two-step deposition process exhibit the FWHM values of 2.61° and 1.73°, respectively.

As shown in Figure 6, two different layers of AlN thin films can be identified using the bright field (BF) TEM image. It is clear that the AlN thin film exhibits numerous columnar grains which are perpendicular to the surface of 3C-SiC. The electron diffraction (ED) patterns of 1-μm-thick AlN film grown on the 3C-SiC/Si substrate along the AlN [110] zone axis are shown in Figure 7. The electron beam size is approximately 300 nm which is large enough to cover many AlN columnar grains shown in Figure 6. This result supports that the AlN grains on the surface of 3C-SiC are well-textured and approximately along the same direction.

B. SAW device on AlN/3C-SiC/Si composite structure

To demonstrate the practical operation of the AlN/3C-SiC/Si composite structure, two different designs of two-port SAW device were fabricated utilizing the lift-off technique. In the composite structure, surface acoustic waves propagate in the plane normal to the *c*-axis of AlN films and along the [001] axis of the 3C-SiC/Si (100) substrates.

Figure 8 is a microscope image of a two-port SAW device consisting of two sets of interdigital transducer (IDT) which was fabricated on the AlN/3C-SiC/Si composite structure. SAW devices with two different designs summarized in Table 2 are used to examine the piezoelectricity of the AlN thin film. The transmission characteristics of the SAW devices were measured using an Agilent E5071B network analyzer. Figure 9 details the measured frequency responses of SAW devices on the AlN/3C-SiC/Si layered structure after time-gating which was employed to remove the feedthrough effect. An expected Rayleigh mode shows a center frequency of 260 MHz while the wavelength is 20 μm. In other words, the Rayleigh mode exhibits a high phase velocity up to 5,200 m/s for 1-μm-thick AlN film and 2.3-μm-thick 3C-SiC film on the Si (100) substrate. This result confirms that the AlN/3C-SiC/Si structure possesses a high acoustic velocity, beneficial for high frequency applications.

Figure 8: The microscope image of the fabricated SAW device (Design 1) on the AlN/3C-SiC/Si composite structure.

Figure 9: Measured frequency responses of SAW devices on the AlN/3C-SiC/Si layered structure after time-gating.

Table 2: Dimensions of SAW Devices.

	Design 1	Design 2
IDT pairs	30	40
Aperture	400 μm	400 μm
Electrode width	5 μm	5 μm
Delay line	400 μm	400 μm
Al electrode thickness	150 nm	150 nm

CONCLUSION

For the first time, the heteroepitaxial AlN (002) thin films were successfully deposited on 3C-SiC(100)/Si(100) substrates using AC reactive magnetron sputtering at temperatures around 300-450 °C. A two-step deposition process is used to overcome the large lattice mismatch of 28.6% between AlN and 3C-SiC. The lowest FWHM value of 1.31° was achieved with a 3- μm -thick heteroepitaxial AlN film, indicating that highly *c*-axis oriented AlN films have been grown on the 3C-SiC/Si substrate. Two-port SAW devices were fabricated on the AlN/3C-SiC/Si composite structure and exhibited the expected Rayleigh mode with an acoustic velocity of 5200 m/s. The results confirm that the AlN/3C-SiC/Si composite structure can be utilized to create RF MEMS devices as well as piezoelectric MEMS sensors and actuators for operation in harsh environments.

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