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Preparation of highly oriented aluminum nitride thin films on molybdenum bottom electrodes using metal interlayers

M. AKIYAMA, N. UENO, H. TATEYAMA
On-Site Sensing and Diagnosis Research Laboratory, National Institute of Advanced Industrial Science and Technology, 807-1 Shuku, Tosu, Saga 841-0052, Japan

K. NAGAO, T. YAMADA
Ube Research Laboratory, Corporate Research & Development, Ube Industries Ltd., 1978-5 Kogushi, Ube, Yamaguchi 755-8633, Japan

We have investigated the influence of metal interlayers on the crystallinity and crystal orientation of aluminum nitride (AlN) thin films prepared on molybdenum (Mo) bottom electrodes. The interlayres were prepared between the Mo bottom electrodes and silicon substrates. Although the sputtering conditions of AlN films and Mo electrodes were the same, the Au/Ti interlayer drastically increased the XRD intensity of the (0002) AlN and (110) Mo planes, and decreased the full width at half maximum (FWHM) of the rocking curves of the (0002) AlN peaks from 9.22° to 3.02°. The Au/Ti interlayers were effective for the improvement in the crystallinity and crystal orientation of AlN films deposited on Mo bottom electrodes. Furthermore, we clarified that the crystallinity and orientation of AlN films and Mo electrodes strongly depend on those of the Au interlayers, and the Au interlayers influence the morphologies of the Mo electrodes.

1. Introduction

Next-generation wireless mobile telecommunications require small size, high power handling and high frequency wireless communication devices [1–4]. Devices based on thin film bulk acoustic wave (BAW) resonator technology provide smaller size, better power handling and higher frequency compared to current surface acoustic wave (SAW) devices. BAW-filters are expected to replace SAW-filters in many applications in the near future [5]. The schematic view of a BAW-filter is shown in Fig. 1 [6]. A BAW resonator consists of a piezoelectric thin film sandwiched by two metal film electrodes. At a certain frequency, a standing wave is formed inside the bulk film, and a maximum output is achieved through electromechanical coupling. The resonance frequency of a BAW resonator is primarily determined by the thickness and material of the piezoelectric layer and electrodes. Both aluminum nitride (AlN) and zinc oxide (ZnO) are the most widely used piezoelectric materials for BAW resonators and filter applications [5]. AlN has higher acoustic wave velocity (11000 m/s for longitudinal waves) and lower dependency on temperature variations than ZnO [7, 8]. Furthermore, in AlN films, low dielectric losses and reasonable electromechanical coupling coefficients can be achieved, if highly oriented AlN films are grown. Therefore most of BAW resonator structures currently under development include AlN piezoelectric layers [1–7, 9].

Highly oriented AlN films are necessary for BAW-filters with high electromechanical coupling [1, 9]. Growth of highly oriented AlN films heavily depends on the material and quality of the bottom electrodes. The functionality of the bottom electrodes is strongly dependent on its uniformity as well as its microstructure. It is desirable to prepare the bottom electrodes with a small surface roughness ($R_{ms} < 5$ nm) and controllable stress in order to prepare highly oriented AlN films. Recent work has focused on molybdenum (Mo) bottom electrodes, because Mo electrodes are easily wet etched and have better acoustic wave propagation property than platinum (Pt) and gold (Au) due to the high acoustic velocity [5]. However, it is reported that AlN films directly deposited on Mo bottom electrodes indicate low crystallinity and low c-axis orientation [2, 10]. Thus, we have pursued sputtering conditions, studying the crucial factors and screening many different metal interlayers in order to improve the crystallinity and crystal orientation of AlN films prepared on Mo electrodes. Consequently, we found that Au/Ti interlayres are effective in improving the crystallinity and orientation of AlN films deposited on Mo electrodes. The present study details the influence of metal interlayers, such as Au/Ti, Ag/Ti and Pt/Ti, on the crystallinity and crystal orientation of AlN films and Mo electrodes.

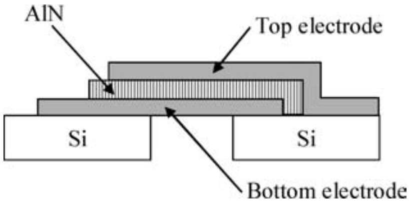

Figure 1 Schematic view of film bulk acoustic resonator (FBAR) using AlN thin film.

2. Experimental procedure

AlN thin films were prepared in a radio frequency planar magnetron sputtering system. The reactive sputtering conditions of AlN films were as follows [11]. The target of AlN films was 76.2 mm.-diam. 99.999% pure aluminum. The base pressure was better than 4×10^{-4} Pa, and then high-purity argon (99.999% purity) and nitrogen (99.999% purity) gases were introduced. The sputtering rate was 5.2 nm/min, and the thickness of the AlN films was 1 μm. Metal thin films were prepared by a d.c. sputtering system of the corresponding metal targets in a high-purity Ar environment at room temperature. The targets were 150 mm.-diam. 99.95% or more pure metals. The sputtering rate of Au, Pt, Ag, Mo and Ti was 120, 75, 172, 39 and 24 nm/min, respectively. The thickness of Mo thin films was 250 nm. The Ti films deposited under gold, silver and platinum films were applied as adhesion layer, and the thickness of Ti films was 30 nm. The metal films were exposed to air before loading into the AlN deposition system. The detailed sputtering conditions of AlN and metal thin films are shown in Table I.

The substrates were (100) silicon wafers with a 1 μm thermal oxide coating. Each substrate was ultrasonically cleaned in ion exchanged water, methanol (99.5% purity) and acetone (99.8% purity) for about 3 min. The targets were cleaned under the sputtering conditions for 5 min, before each deposition. The crystal structure and crystallinity of AlN films and metal interlayers were examined by X-ray diffraction (XRD) using Cu K_α radiation. Their crystal orientations were evaluated by the full width at half maximum (FWHM) of the X-ray rocking curves of the films and electrodes. The surface roughness was measured by using an atomic force microscope (AFM).

3. Results and discussions

We prepared Au/Ti interlayers between Mo bottom electrodes and silicon substrates, Mo/Au/Ti/SiO_2/Si, in order to prevent molybdenum-silicide formation,

TABLE I Sputtering conditions of AlN and metal thin films

Material	AlN	Metal
Sputtering system	RF	DC
Power	325 W	150 W
Substrate temperature	300°C	R.T.
Sputtering pressure	0.5 Pa	0.5 Pa
Atmosphere	Ar:N_2 = 1:1	Ar
Rf frequency	13.56 MHz	–
Target substrate spacing	>8.3 cm	6.5 cm

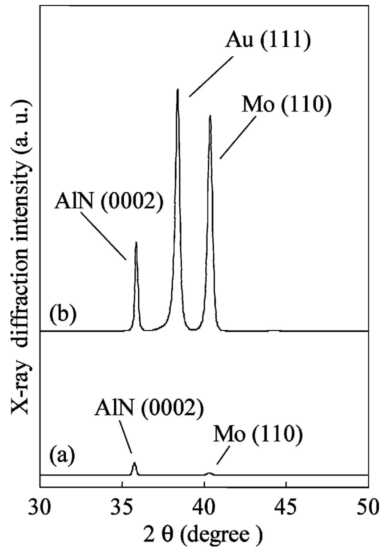

Figure 2 X-ray diffraction patterns of AlN thin films: (a) prepared on Mo electrode and (b) prepared on Mo/Au/Ti electrode. The film thickness of Au layer was 100 nm.

because it is known that Mo thin films react with silicon substrates at high temperature [12–14]. We investigated the influence of the interlayers on the crystallinity and crystal orientation of AlN films and Mo bottom electrodes. Fig. 2 shows the X-ray diffraction (XRD) patterns of AlN films prepared on Mo/SiO_2/Si and Mo/Au/Ti/SiO_2/Si substrates, respectively, under the same sputtering conditions. Fig. 2a shows that two peaks are observed at 35.99° and 40.56°, and they are indexed as hexagonal (0002) AlN and (110) Mo plane diffraction peaks [2, 10, 15]. The preferential orientations of the AlN film and Mo electrode were (0002) and (110) respectively, however the corresponding peak intensities were quite low. These results are in agreement with those reported by Lee *et al.* [2] and Takikawa *et al.* [10], indicating that it is difficult to prepare highly oriented AlN films on Mo bottom electrodes directly. On the other hand, when the Au/Ti interlayer was used, well-defined peaks appeared at 35.99°, 38.50° and 40.56°, like shown in Fig. 2b, and they are indexed as hexagonal (0002) AlN, (111) Au and (110) Mo plane peaks [2, 10]. The peak intensity of the AlN film and Mo electrode drastically increased, suggesting that the crystallinity of the AlN film and Mo electrode was significantly improved by the interlayer. It should be noted that the crystallinity of the Mo electrode was also increased by the interlayer. Fig. 3 shows the X-ray rocking curves of the (0002) AlN plane peaks. The FWHM of the rocking curves was 9.22° and 3.02°, respectively. The FWHM decreased by the interlayer, revealing that the crystal orientation of the AlN films was also drastically improved by the interlayer. From these results, Au/Ti interlayers are effective for the improvement in the crystallinity and crystal orientation of AlN films deposited on Mo bottom electrodes.

In addition, we investigated the influence of Ag/Ti and Pt/Ti interlayers on the crystallinity and crystal orientation of AlN films and Mo electrodes in order to evaluate that of Au/Ti interlayers. Because it is known that the crystallinity and crystal orientation of Au/Ti,

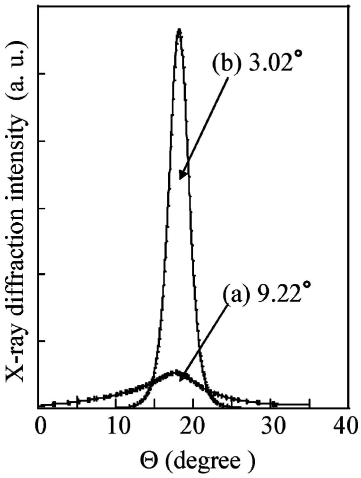

Figure 3 X-ray diffraction patterns of AlN thin films: (a) prepared on Mo electrode and (b) prepared on Mo/Au/Ti electrode. The film thickness of Au layer was 100 nm.

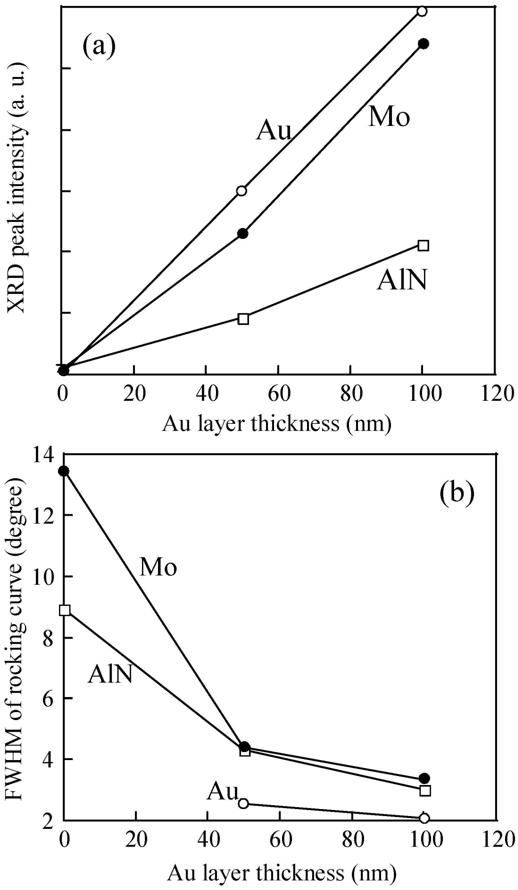

Figure 4 (a) Dependence of XRD peak intensity of AlN, Mo and Au films on Au layer thickness, for AlN (□), Mo (●) and Au (○). b) Dependence of FWHM of X-ray rocking curves of AlN, Mo and Au films on Au layer thickness, for AlN (□) Mo (●) and Au (○). The film thickness of Mo and AlN films was 250 nm and 1 μm.

Ag/Ti and Pt/Ti films are comparatively high [16]. As presented in Table II, the X-ray diffraction intensity of AlN/Mo/Au/Ti film was the highest in the present study. The crystallinity of the AlN film prepared on the Mo/Au/Ti bottom electrode was the best. Furthermore, the FWHMs of X-ray rocking curves of the AlN films prepared on the Mo/Ag/Ti and Mo/Pt/Ti electrodes were 5.61° and 6.05°, respectively. The AlN film prepared on the Mo/Au/Ti electrode exhibited the lowest FWHM, indicating that the Au/Ti interlayer was more effective for the improvement in the crystallinity and crystal orientation. The surface roughness of the Au/Ti, Ag/Ti and Pt/Ti interlayers was 1.08, 4.20 and 2.54 nm, respectively, and the crystal orientation of the AlN films deposited on them did not depend on the surface roughness.

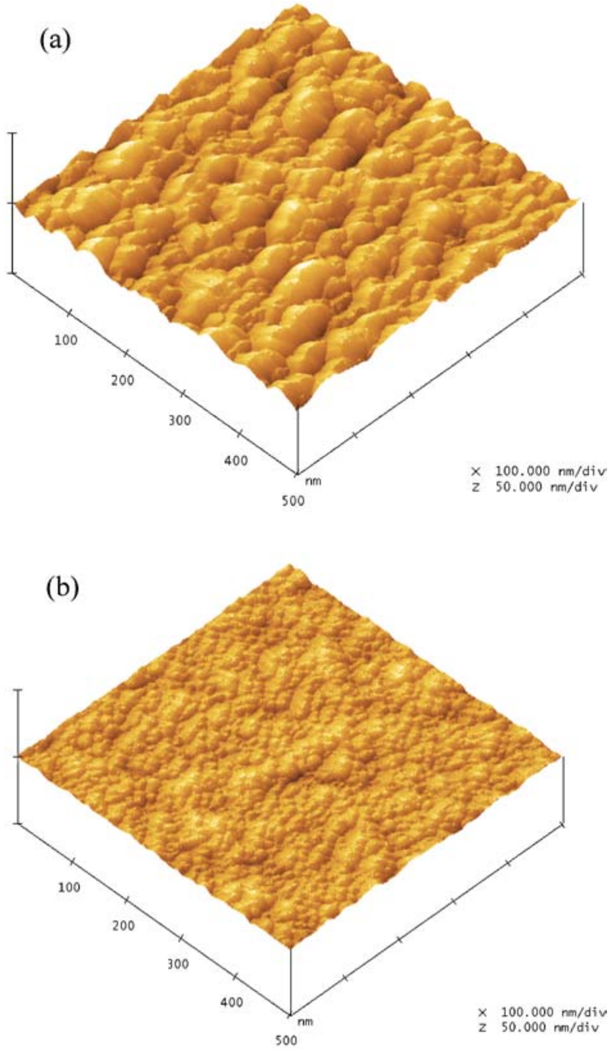

Figure 5 AFM surface images of Mo electrodes prepared (a) without Au/Ti interlayer and (b) with Au/Ti interlayer.

We studied the dependence of the XRD peak intensity of AlN films and Mo electrodes prepared on Au/Ti interlayers on the film thickness of the Au layers. The result is shown in Fig. 4a. Although the sputtering conditions of the AlN film and Mo electrode were the same, the peak intensity of the AlN and Mo increased with

TABLE II Influence of bottom electrodes on crystallinity and crystal orientation of AlN thin films

Electrode	Mo	Mo/Au/Ti	Mo/Ag/Ti	Mo/Pt/Ti
Intensity (cps)	970	11096	4881	5082
FWHM (deg.)[a]	9.22	3.02	5.61	6.05
Surface roughness of interlayer (nm)	–	1.08	4.20	2.54

[a]FWHM is the full width at half-maximum of the X-ray rocking curves of the A1N films.The film thickness of Mo, Au, Ag and Pt films was 250 nm, 100 nm, 100 nm and 100 nm, respectively.

increasing the Au layer thickness. The Au layer thickness strongly affected the crystallinity of the AlN film and Mo electrode. Fig. 4b shows the dependence of the FWHM of rocking curves of the (0002) AlN, (110) Mo and (111) Au plane peaks on the Au layer thickness. All the FWHMs decreased with increasing the Au layer thickness. Lee *et al.* [2] and Jakkaraju *et al.* [17] reported that AlN texture improves with an improvement in electrode texture. We think that the crystallinity and crystal orientation of the AlN film and Mo electrode are improved by the high crystallinity and crystal orientation of the Au layer.

To compare the microstructures of Mo bottom electrodes, we measured the surface morphologies of Mo electrodes grown on Si substrate and Au/Ti interlayer. Fig. 5 shows the atomic force microscopy (AFM) images of the surface morphologies. The surface feature of the Mo electrode directly deposited on the Si substrate was comparatively rough (Surface roughness $R_{ms} = 2.22$ nm), and was formed by large nanoparticles (Fig. 5a). Whereas the surface feature of the Mo/Au/Ti electrode was smooth ($R_{ms} = 0.75$ nm), and was formed by fine nanoparticles, like shown in Fig. 5b. From these results, we think that the Au/Ti interlayer prevents the growth of Mo grains, and decreases the surface roughness of the Mo electrodes. The smooth surface is beneficial for highly oriented AlN film growth [2, 17].

4. Conclusions

We have investigated the influence of metal interlayers on the crystallinity and crystal orientation of AlN thin films prepared on Mo bottom electrodes. The crystallinity and crystal orientation of the AlN films and Mo electrodes were significantly improved by metal interlayers. Au/Ti interlayers were more effective than Ag/Ti and Pt/Ti interlayers. The crystallinity and orientation of AlN films and Mo electrodes strongly depended on those of the Au layers in Au/Ti interlayers. Furthermore, we consider that Au/Ti interlayer prevents the growth of Mo grains, and decreases the surface roughness of the Mo electrodes, therefore, the smooth surface is beneficial for highly oriented AlN film growth.

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