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# Improvement in crystal orientation of AlN thin films prepared on Mo electrodes using AlN interlayers

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#### **Abstract**

Highly c-axis oriented aluminum nitride (AlN) thin films have been prepared on molybdenum (Mo) bottom electrodes using AlN interlayers (AlN-IL), by reactive rf magnetron sputtering. The interlayers were deposited between the Mo electrodes and silicon substrates, such as AlN/Mo/AlN-IL/Si. The crystallinity and crystal orientation of the interlayers depend on the interlayer thickness and strongly influence those of the Mo electrodes and AlN films. From transmission electron microscopy observations and X-ray pole figure measurements, the interlayer, Mo electrode and AlN film consist of columnar grains and exhibit a fiber texture. It has been found that they have the local epitaxial relationship of  $(0\,0\,0\,1)$  [2  $\bar{1}$   $\bar{1}$  0] AlN-IL/ $/(1\,1\,0)$ [ $\bar{1}$  1 1] Mo/ $/(0\,0\,0\,1)$  [2  $\bar{1}$   $\bar{1}$  0] AlN. The nucleation process of AlN thin films changes from a fine grain structure to a columnar structure.

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#### 1. Introduction

The rapid advancement of mobile communications has required high frequency band-pass filters. Film bulk acoustic resonator (FBAR) filters are well suited for mobile communication systems operating at high frequencies in the GHz range. In FBAR filters, the total thickness, electromechanical coupling coefficient and acoustic material quality determine the operating frequency, bandwidth and insertion loss, respectively.

Aluminum nitride (AlN) is one of the most promising candidates as a piezoelectric material for FBAR, because AlN has a high bulk acoustic wave velocity, a high electrical resistance, a wide band gap and compatibility with silicon processing [1]. AlN has a wurtzite crystal structure with *a*-axis of 0.3112 nm and *c*-axis of 0.4982 nm [2]. If highly *c*-axis oriented AlN films are grown, the high electromechanical coupling coefficient and low loss can be achieved. In addition, it is

important to select bottom electrode materials in FBAR, because the acoustic waves generated pass through an entire resonating stack. AlN films preferentially grow in the c-axis on various metal electrodes, such as (1 1 1) Pt, (1 1 1) Au and (1 1 1) Al electrodes due to the lattice match [3]. However, Pt and Au electrodes are difficult to deposit directly on substrates and to be etched out. Al electrodes also have problems of surface oxidation and etching selectivity with AlN. Molybdenum (Mo) has some superior properties as FBAR electrodes, because it has low acoustic attenuation, high electrical conductivity, high adhesion strength with AlN and good etching capability [4]. Although Mo electrodes have such clear advantages, it is difficult to prepare highly crystal oriented AlN films on Mo bottom electrodes. Recently, a few researchers have successfully prepared highly oriented AlN films on polycrystalline Mo bottom electrodes by optimizing the reactive sputtering conditions [4,5].

In this work, the crystal growth of highly c-axis oriented AlN films on Mo bottom electrodes was investigated using AlN interlayers (AlN-IL) between the electrodes and silicon substrates, such as AlN/Mo/AlN-IL/Si. Furthermore the microstructure of the films was analyzed and the crystal-

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lographic relationship between the AlN and Mo films was revealed.

#### 2. Experimental procedure

AlN interlayers, Mo electrodes and AlN films were prepared on (1 0 0) Si substrates in a rf magnetron sputtering system (CFS-4ES, Tokuda). The distance between the target and substrate was more than 83 mm. The vacuum chamber was evacuated below  $2 \times 10^{-4}$  Pa. The AlN interlayers and AlN films were deposited at 300 °C in 0.5 Pa reactive Ar/N<sub>2</sub> gas mixtures, where the N<sub>2</sub> concentration was 50%. The rf discharge power was 400 W. The target was 3-in. diameter Al (99.999%), and was pre-cleaned at the same deposition condition for 10 min with the shutter closed, before the deposition process commenced. The interlayer thickness altered from 0 to 200 nm, and the thickness of the AlN films was 1 µm. The Mo electrodes were deposited in 0.3 Pa Ar gas and with a power of 100 W. The target was 3-in. diameter Mo (99.9%), and was pre-cleaned at the same deposition condition for 5 min with the shutter closed before the deposition process. The Mo electrode thickness was 200 nm. The crystal structure and crystallinity of the films were examined using Xray diffraction (XRD: M03X-HF, Mac Science) with Cu Kα radiation. The crystal orientation was evaluated from the fullwidth at half-maximum (FWHM) of X-ray rocking curves. The in-plane alignment was examined by the X-ray pole figure method (X'Pert-MRD with 4 circle goniometer, Philips). The microstructure was observed by transmission electron microscopy (TEM: JEM-2000EX) operated at 200 kV. TEM samples were prepared with a focused ion beam mill (FB-2000K, Hitachi).

#### 3. Results and discussion

The influence of AlN interlayers on the crystallinity and crystal orientation of AlN films deposited on Mo bottom electrodes was investigated. Fig. 1 shows the XRD patterns of AlN films deposited on (a) Mo/Si and (b) Mo/AlN-IL/Si substrates. Only two peaks due to (0 0 0 2) AlN and (1 1 0) Mo planes were observed in the XRD patterns. Although the deposition conditions of the AlN and Mo were the same, the peak intensities of the AlN film and Mo electrode prepared on the interlayer were 40 times higher than those of the AlN film and Mo electrode directly deposited on the Si substrate. This result indicates that the crystallinity of the AlN film and Mo electrode is significantly improved by the AlN interlayer. The inset of Fig. 1 shows the X-ray rocking curves of the (0 0 0 2) AlN peaks. The FWHM of the rocking curves decreases from 9.1° to 2.5° using the AlN interlayer. This result suggests that the crystal orientation of the AlN film is also improved by the AlN interlayer.

The dependence of the peak intensity of XRD and FWHM of X-ray rocking curves of the AlN interlayers, Mo electrodes and AlN films on the interlayer thickness was investigated in order to clarify the influence of the interlayer thickness on the crystallinity and crystal orientation of the AlN interlayers, Mo electrodes and AlN films. Fig. 2 shows the dependence of the peak intensity of the AlN interlayers, Mo electrodes and AlN

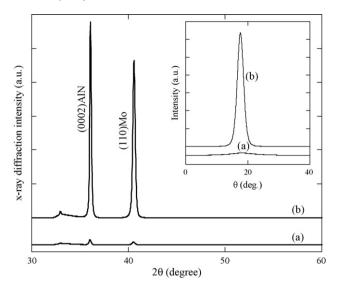


Fig. 1. X-ray diffraction patterns of AlN films prepared on Mo electrodes (a) without an AlN interlayer and (b) with an AlN interlayer. The inset shows the rocking curves of the  $(0\ 0\ 0\ 2)$  AlN. The thickness of AlN interlayers, Mo electrodes and AlN films were  $200\ nm$ ,  $200\ nm$  and  $1\ \mu m$ , respectively.

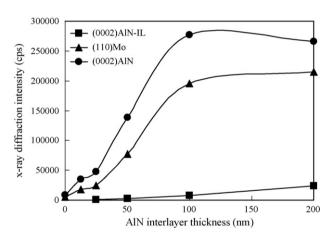


Fig. 2. Dependence of peak intensity of AlN interlayers ( $\blacksquare$ ), (1 1 0) Mo electrodes ( $\triangle$ ) and (0 0 0 2) AlN films ( $\bigcirc$ ) on AlN interlayer thickness.

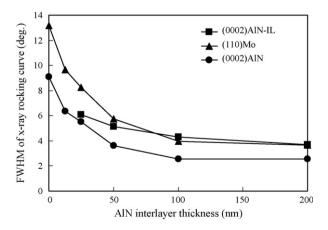


Fig. 3. Dependence of FWHM of X-ray rocking curves reflected from (0 0 0 2) AlN interlayers ( $\blacksquare$ ), (1 1 0) Mo electrodes ( $\blacktriangle$ ) and (0 0 0 2) AlN films ( $\bullet$ ) on AlN interlayer thickness.

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