# **Evaluation of Piezoelectric Ta<sub>2</sub>O<sub>5</sub> Thin Films Deposited on Ta Oxide Film**

Ta酸化膜上への圧電性 Ta<sub>2</sub>O<sub>5</sub>薄膜の成膜と評価

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## 1. Introduction

An X-axis-oriented tantalum pentoxide  $(Ta_2O_5)$  piezoelectric thin film has a strong piezoelectric property and a high dielectric constant.<sup>1</sup> However, there is a problem that a large propagation loss for the Rayleigh-type SAW (R-SAW) or bulk wave occurs in the oriented  $Ta_2O_5$  thin films.<sup>2,3</sup>

By utilizing the single crystallization of  $Ta_2O_5$ thin films, a reduction in propagation loss can be expected. In the deposition of Ta<sub>2</sub>O<sub>5</sub> thin films using an RF magnetron sputtering system with a long-throw sputter (LTS) cathode, we repoted that a hexiagonal Ta<sub>2</sub>O<sub>5</sub> (called the  $\delta$  phase,  $\delta$ -Ta<sub>2</sub>O<sub>5</sub><sup>4</sup>) thin film with (203) orientation was produced on c-plane sapphire  $(c-Al_2O_3)$  by epitaxial growth.<sup>5</sup> However, since  $\delta$ -Ta<sub>2</sub>O<sub>5</sub> belongs to the 6/mmm point group without piezoelectricity, no increase in coupling factor and no major improvement in propagation loss were observed.<sup>5</sup> On the other hand, Gnanarajan and Lam reported that an epitaxial orthorhombic twinned Ta<sub>2</sub>O<sub>5</sub> film with (201) orientation was fabricated by the low-pressure thermal oxidation of epitaxial tantalum (Ta) films on the R-plane of sapphire  $(R-Al_2O_3)$  substrates.<sup>6</sup> However, the piezoelectricity and SAW properties were not evaluated.

In this study, for the R-Al<sub>2</sub>O<sub>3</sub> substrate, homoepitaxial growth of the Ta<sub>2</sub>O<sub>5</sub> thin film using an oxide Ta thin film (TaO<sub>x</sub>) as a buffer layer was examined, and the crystalline and R-SAW propagation properties of the thin films were evaluated.

## 2. Sample Fabrication

The sample was fabricated using the RF magnetron sputtering system. First, a metal Ta thin film with a thickness of 70 nm was deposited on the R-Al<sub>2</sub>O<sub>3</sub> substrate in an atmosphere gas of only Ar (30 ccm) at 700 °C, and the metal Ta thin film was oxidized in the chamber in an atmosphere gas of Ar and O<sub>2</sub> (30:10 ccm) for 10 min at 700 °C. Next, the Ta<sub>2</sub>O<sub>5</sub> film was deposited on the TaO<sub>x</sub> thin film for 6 h at 700 °C under similar sputtering conditions to those in the previous report<sup>5</sup>. The total film thickness *h* was 3.0 µm.



Fig. 1 XRD patterns of  $Ta_2O_5$  thin films deposited on  $TaO_x/R-Al_2O_3$ ,  $R-Al_2O_3$ ,  $c-Al_2O_3$ .

## 3. Evaluation of Crystallization

First, the degree of orientation was evaluated from X-ray diffraction (XRD) patterns using a CuK $\alpha$  X-ray source. **Figure 1** shows the XRD pattern of the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample and the plane directions of orthorhombic Ta<sub>2</sub>O<sub>5</sub> (called the  $\beta$  phase,  $\beta$ -Ta<sub>2</sub>O<sub>5</sub>). For comparison, the XRD patterns of the Ta<sub>2</sub>O<sub>5</sub> thin films with *h* of 3.0 µm deposited on *R*-Al<sub>2</sub>O<sub>3</sub> and *c*-Al<sub>2</sub>O<sub>3</sub> substrates without buffer layer using the same sputtering conditions (800 °C) were also shown in Fig. 1.

The preferential (200) orientation was observed for each sample. On the other hand, for the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample, a peak at approximately  $2\theta$ =37° was observed. There was no peak at approximately 37° for the Ta<sub>2</sub>O<sub>5</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample without buffer layer. A peak at approximately 37° of the Ta<sub>2</sub>O<sub>5</sub>/*c*-Al<sub>2</sub>O<sub>3</sub> sample without buffer layer corresponds to the diffraction angle of the (203) plane of the  $\delta$ -Ta<sub>2</sub>O<sub>5</sub>.<sup>5</sup>

Next, the in-plane crystallinity of the  $Ta_2O_5$ thin film was evaluated from transmission electron microscopy (TEM) diffraction patterns. **Figure 2** shows the TEM patterns. The *R*-Al<sub>2</sub>O<sub>3</sub> sample with the TaO<sub>x</sub> buffer layer was observed like a four-fold symmetry pattern [Fig. 2(a)]. It was different from the *R*-Al<sub>2</sub>O<sub>3</sub> sample without buffer layer, in which a ring-shape pattern was observed [Fig. 2(b)]. Therefore, there is a possibility that a part of the Ta<sub>2</sub>O<sub>5</sub> film was crystallized by using the TaO<sub>x</sub> buffer layer.

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Fig. 2 TEM patterns of  $Ta_2O_5$  thin films deposited on (a)  $TaO_x/R-Al_2O_3$ , (b)  $R-Al_2O_3$ , (c)  $c-Al_2O_3$ .

On the other hand, the pattern of the *R*-Al<sub>2</sub>O<sub>3</sub> sample with buffer layer was also different from the *c*-Al<sub>2</sub>O<sub>3</sub> sample, in which a six-fold symmetric pattern was observed [Fig. 2(c)]. Furthermore, the peak at approximately 37° in the XRD pattern of the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample in Fig. 1 corresponds to the diffraction angle of the (111) and (201) planes of the  $\beta$ -Ta<sub>2</sub>O<sub>5</sub> (2 $\theta$ =36.67°, 37.05°).

From the above results, the possibility of the homoepitaxial growth of the  $\beta$ -Ta<sub>2</sub>O<sub>5</sub> on TaO<sub>x</sub> buffer layer was demonstrated. However, from the bright-field image obtained by TEM, a polycrystalline structure with various grain sizes was observed in the Ta<sub>2</sub>O<sub>5</sub> thin film of the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample.

### 4. Evaluation of SAW Properties

Interdigital transducers (IDTs) with a period  $\lambda$  of 20 µm and 30 double-finger pairs were fabricated on the deposited film using an Al film so that the SAW propagation direction could be set as the *Y*-axis of Al<sub>2</sub>O<sub>3</sub>, namely, *R*-*Y* and *Z*-*Y* (*c*-plane) Al<sub>2</sub>O<sub>3</sub>. The propagation length between the center of the input and that of the output IDT was 80  $\lambda$ .

The frequency responses of each sample with  $h/\lambda=0.150$  measured using a network analyzer were shown in **Fig. 3**. The zeroth and first modes of the R-SAW were observed for the each sample. The insertion loss *IL* of the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample was significantly larger than those of the samples without the TaO<sub>x</sub> buffer layer because the Ta<sub>2</sub>O<sub>5</sub> thin film deposited on the TaO<sub>x</sub> buffer layer was a polycrystalline thin film.

**Figure 4** shows the coupling factor  $K^2$  measured from the admittance of the IDT. For the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-Al<sub>2</sub>O<sub>3</sub> sample, the enhancement of  $K^2$  can be expected because  $\beta$ -Ta<sub>2</sub>O<sub>5</sub> must have piezoelectricity. However, as also shown in Fig.4, the  $K^2$  values of the Ta<sub>2</sub>O<sub>5</sub>/TaO<sub>x</sub>/*R*-*Y* Al<sub>2</sub>O<sub>3</sub> sample with  $h/\lambda=0.150$  were approximately half that of the Ta<sub>2</sub>O<sub>5</sub>/*R*-*Y* sample. This was considered to be due to the polycrystalline structure of the Ta<sub>2</sub>O<sub>5</sub> thin film on the TaO<sub>x</sub> buffer layer.

On the other hand, for the first modes on *R*-*Y* and *Z*-*Y* Al<sub>2</sub>O<sub>3</sub> samples, the value of  $K^2$  of 1.8 % and the phase velocity of approximately 5,000 m/s were obtained at  $h/\lambda=0.225$ . Furthermore, it was found that the Ta<sub>2</sub>O<sub>5</sub>/*R*-*Y* Al<sub>2</sub>O<sub>3</sub> samples had a



larger  $K^2$  than the Ta<sub>2</sub>O<sub>5</sub>/*Z*-*Y* Al<sub>2</sub>O<sub>3</sub> samples. This is because the *X*-axis-oriented Ta<sub>2</sub>O<sub>5</sub> thin film and the (203)-oriented  $\delta$ -Ta<sub>2</sub>O<sub>5</sub> thin film were mixed in the deposited thin film on the *Z*-*Y* Al<sub>2</sub>O<sub>3</sub> substrate.

#### 5. Conclusion

For the *R*-Al<sub>2</sub>O<sub>3</sub> substrate, homoepitaxial growth of the Ta<sub>2</sub>O<sub>5</sub> thin film using the TaO<sub>x</sub> buffer layer was examined, and the crystalline and R-SAW propagation properties of the thin films were evaluated. The possibility that a part of the Ta<sub>2</sub>O<sub>5</sub> film was crystallized to the orthorhombic  $\beta$ -Ta<sub>2</sub>O<sub>5</sub> with piezoelectricity due to the homoepitaxial growth was demonstrated. Unfortunately, no major improvement in propagation properties was observed upon the crystallization because the Ta<sub>2</sub>O<sub>5</sub> thin film on the TaO<sub>x</sub> buffer layer was polycrystalline structure.

#### References

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