Evaluation of Ta₂O₅ Piezoelectric Thin Film Prepared on Pt/Si Substrate at Low Deposition Rate

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1. Introduction

With the shift of mobile communication systems to higher frequencies and wider bandwidths, piezoelectric materials with higher velocity, higher coupling factor (K^2), and lower loss are required for the development of high-performance frequency filters using surface acoustic waves (SAWs) and bulk acoustic waves (BAWs). An *X*-axis-oriented tantalum pentoxide (Ta₂O₅) piezoelectric thin film fabricated by sputtering has piezoelectricity comparable to that of ZnO thin films and high dielectric constant¹. The methods of depositing single-crystal Ta₂O₅, which is expected to have a higher K^2 and a lower propagation loss than the oriented thin film, have been investigated.

We deposited Ta₂O₅ thin films on platinum (Pt)/Si and strontium ruthenate (SrRuO₃) substrates (SRO/Pt/Si substrate) using an RF magnetron sputtering system. From the pole figure plots, we determined that λ -Ta₂O₅ without piezoelectricity grew on the Pt/Si substrate and that β -Ta₂O₅ with piezoelectricity grew on the SRO/Pt/Si substrate. In addition, the Ta₂O₅ thin film was crystallized to a greater extent at a lower deposition rate (0.4 µm/h). The Ta₂O₅ thin film formed at a normal deposition rate (0.8 µm/h) to a film thickness of 6.5 µm was dominated by the *X*-axis-oriented film and exhibited a larger k_t^2 than the epitaxial film².

In this study, we examined the crystal structure and bulk acoustic wave (BAW) propagation properties of Ta_2O_5 thin films prepared at low deposition rates on Pt/Si and SRO/Pt/Si substrates.

2. Deposition of Ta_2O_5 thin films and evaluation of crystallinity

Ta₂O₅ thin films were deposited on Pt(100)/Si and SRO/Pt/Si substrates using an RF magnetron sputtering system¹ at a substrate temperature of 700°C (thickness h_t : 7.0 µm). The degree of orientation of the samples was evaluated from X-ray diffraction (XRD) patterns. The XRD patterns measured for the two samples are shown in **Fig. 1**. For both samples, the preferential orientation of monoclinic Ta₂O₅(100) was observed. However, the Ta₂O₅/Pt/Si sample shows a weak peak near 37°, which was not observed for the X-axis-oriented Ta₂O₅ films, indicating that the Ta₂O₅ epitaxial thin film was grown governed by the lattice plane of Pt, as in the case of the normal deposition rate². On the other hand, for the $Ta_2O_5/SRO/Pt/Si$ sample, no peak was observed around 37°, and the growth of an epitaxial film could not be determined from the XRD pattern.

Then, the fluctuation of the plane orientation was evaluated by measuring rocking curves using the same X-ray diffractometer. The measured rocking curves of the two samples are shown in Fig. 2. The full widths at half-maximum (FWHMs) corresponding to the $Ta_2O_5(200)$ peak for the Ta₂O₅/Pt/Si and Ta₂O₅/SRO/Pt/Si samples were 4.9° and 6.9°, respectively, which are smaller than those of the X-axis-oriented Ta₂O₅ films. Therefore, there is the possibility of the growth of epitaxial film in both samples, as in the case of the normal deposition rate².

The in-plane crystallinity of the Ta₂O₅ thin films was evaluated on the basis of pole figure plots. The diffraction angle 2 θ of the multipurpose X-ray diffractometer was set to 37°. The measured pole figures of the two samples are shown in **Fig. 3**. The peaks were observed on the same circumference at the tilt angles χ =40° and 69°. These peaks correspond to β -Ta₂O₅(201) and β -Ta₂O₅(111)³, respectively. The peak intensity at h_t =7.0 µm was higher than that at h_t =2.6 µm, indicating that crystallinity improves with increasing film thickness, unlike in the case of at the normal deposition rate.



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Fig. 2 Measured rocking curves of $Ta_2O_5/Pt/Si$ and $Ta_2O_5/SRO/Pt/Si$ samples.



Fig. 3 Measured pole figures of $Ta_2O_5/Pt/Si$ and $Ta_2O_5/SRO/Pt/Si$ samples.

3. Evaluation of BAW propagation property

The properties of high-overtone bulk acoustic resonators (HBARs) were evaluated. The HBAR evaluated had a top electrode of Au film deposited on the above samples and a bottom electrode of Pt. The measured conversion loss and the theoretical value after equivalent circuit fitting of HBARs are shown in **Fig. 4**. **Table I** shows the phase velocity (ν) and electromechanical coupling factor (k_t^2) values determined by fitting a theoretical curve calculated using Mason's equivalent circuit model⁴.

v was 5,200 m/s for both samples, and k_t^2 values were 0.96% and 1.44% for the Ta₂O₅/Pt/Si and Ta₂O₅/SRO/Pt/Si samples, respectively. Both k_t^2 values were larger than that of the Ta₂O₅/SRO/Pt/Si sample deposited at a normal rate, in which the *X*-axis-oriented film was dominant. The larger k_t^2 with improved crystallinity suggested that a film mainly composed of β-Ta₂O₅ was deposited.



4. Conclusions

The piezoelectric Ta_2O_5 thin films were deposited on Pt/Si and SRO/Pt/Si substrates at low rates using an RF magnetron sputtering system. The orientation and BAW propagation properties were evaluated.

For low deposition rates, β -Ta₂O₅ grew on both Pt/Si and SRO/Pt/Si substrates. In both cases, the crystallinity improved with increasing film thickness. This result was different from the films deposited at normal deposition rate: λ -Ta₂O₅ grew on the Pt/Si and X-axis-oriented Ta₂O₅ became dominant on SRO/Pt/Si substrate in thicker films.

The evaluated results of HBAR response indicated that the epitaxially grown β -Ta₂O₅ films deposited at a low deposition rate exhibited larger k_t^2 values than those of the samples with X-axisorientation owing to the higher crystallinity.

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References

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Table I BAW propagation properties of Ta₂O₅/Pt/Si and Ta₂O₅/SRO/Pt/Si samples.

Sample	Deposition rate	Ta ₂ O ₅ film thickness	Phase velocity v [m/s]	Electromechanical coupling factor k_t^2 [%]
Ta ₂ O ₅ /Pt/Si	Low	7.0	5,200	0.96
Ta ₂ O ₅ /SRO/Pt/Si	Low	7.0	5,200	1.44
Ta ₂ O ₅ /SRO/Pt/Si ²	Normal	6.5	5,000	0.56