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Deposition and Evaluation of Ta_2O_5 Piezoelectric Thin Film on Pt Crystal Film

Pt 結晶膜上への Ta_2O_5 圧電薄膜の成膜と評価

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1. Introduction

For the recent rapid development of mobile communication devices such as smart phones, high-performance frequency filters using surface acoustic waves (SAWs) and bulk acoustic waves (BAWs) are required. An *X*-axis-oriented tantalum pentoxide (Ta_2O_5) piezoelectric thin film fabricated by sputtering has piezoelectricity comparable to that of ZnO thin films,[1] and a methods of depositing single-crystal Ta_2O_5, which is expected to have a higher electromechanical coupling factor (K^2) and a lower propagation loss than the oriented thin film.

In this study, we examined the epitaxial growth of single-crystal Ta_2O_5 films. We used platinum (Pt) crystal films deposited on Si substrates because the lattice constant of Pt is close to that of orthorhombic Ta_2O_5 (β-Ta_2O_5), which has piezoelectricity and pyroelectricity.[2] In addition, by utilizing high-density Pt, we can expect the concentration of displaced SAW particles, which leads to an increase in K^2. We simulated the SAW resonance properties on the *X*-axis-oriented Ta_2O_5 thin film deposited on the Pt/Si substrate.

2. Deposition of Ta_2O_5 thin films and evaluation of crystallinity

Ta_2O_5 thin films were deposited on a Si substrates with Pt(100) crystal film and Si substrates using an RF magnetron sputtering system[2] at substrate temperatures T_S of 700–750°C (thickness h_t: 1.8–3.1 μm). The degree of orientation of the samples was evaluated from X-ray diffraction (XRD) patterns obtained using a Cu Kα X-ray source. The XRD patterns of the samples measured at T_S of 700°C are shown in **Fig. 1**.

For both samples, the preferential orientation of monoclinic Ta_2O_5(200) was observed. However, for the Pt/Si sample, a peak near 37° appeared, which was not observed for the Si sample. There is a possibility that the Ta_2O_5 crystal thin film that senses the lattice plane of Pt grows. The in-plane crystallinity of the Ta_2O_5 thin films was evaluated on the basis of pole figure plots. The diffraction angle 2θ of a multipurpose X-ray diffractometer was set to 28° and 37°. The measured pole figures of the samples at a substrate temperature of 700°C are shown in **Fig. 2**. The peaks were observed on the same circumference at the tilt angles χ=35° and 60° when 2θ=28° and χ=48° when 2θ=37°; these peaks to correspond to λ-Ta_2O_5(120), λ-Ta_2O_5(011) and λ-Ta_2O_5(220), respectively.[3] The same results were obtained for a sample prepared at a substrate temperature of 750°C.

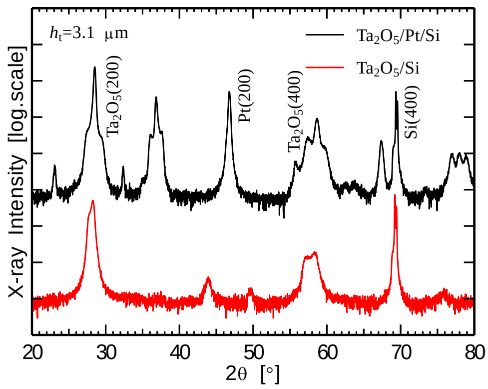

Fig. 1 XRD patterns of Ta_2O_5 thin films.

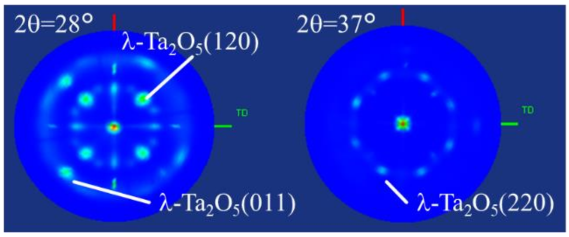

Fig. 2 Measured pole figures of Ta_2O_5/Pt/Si sample.

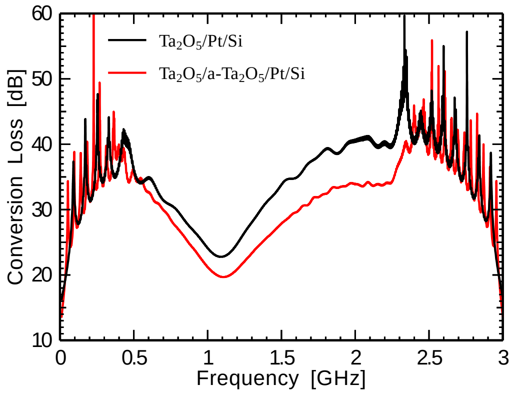

Fig. 3 Frequency responses of HBARs.

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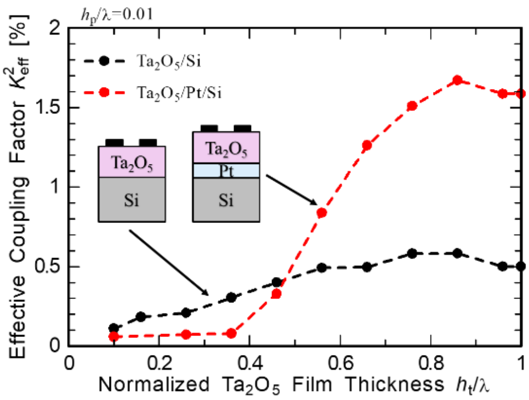

Fig. 4 Simulated K^2_{eff} as a function of film thickness of Ta_2O_5/Si and Ta_2O_5/Pt/Si structures.

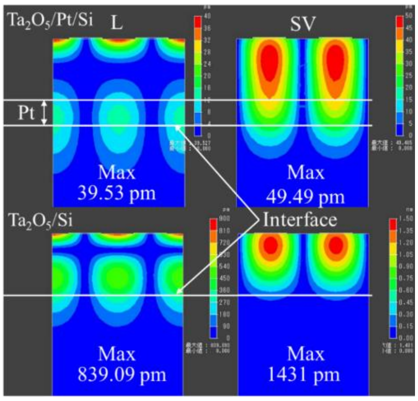

Fig. 5 Simulated particle displacements (h_t/λ=0.46 and h_p/λ=0.2).

3. Evaluation of BAW propagation property

Ta_2O_5 thin films were deposited on a-Ta_2O_5/Pt/Si, in which an amorphous Ta_2O_5 thin film (a-Ta_2O_5) of less than 0.1 μm thickness was deposited as a buffer layer on Pt/Si substrate, and on Pt/Si substrate at a substrate temperature 700°C (h_t: 2.0 μm). It can be expected that the Ta_2O_5 thin film cannot sense the Pt lattice plane owing to the buffer layer. As a result of deposition, the Pt lattice plane was sensitized even with the buffer layer; however, it was confirmed by XRD analysis that sensitivity was suppressed.

The properties of high-overtone bulk acoustic resonators (HBARs) were evaluated using Au film deposited on these samples as the top electrode and Pt as the bottom electrode. The frequency responses of HBARs are shown in **Fig. 3**. Phase velocity and electromechanical coupling factor (k_t^2) were determined by equivalent circuit fitting. The phase velocities were 5,450 m/s and 6,100 m/s, and the k_t^2 values were 0.144% and 0.032%, for samples with and without a-Ta_2O_5 thin film, respectively. The Pt-lattice-plane-insensitive a-Ta_2O_5/Pt/Si sample had a larger k_t^2. We considered that the piezoelectricity of the Pt/Si sample is smaller than that of the Pt-lattice-plane-insensitive sample because λ-Ta_2O_5 has a crystal structure without piezoelectricity.

4. Simulation of SAW resonance property

The finite element method (FEM) was used to analyze the SAW resonance properties of models composed of an infinite periodic interdigital transducer (IDT) on Ta_2O_5/Pt/Si structures. The IDT wavelength λ was 8 μm, the normalized film thickness of Pt (h_p/λ) was 0.01, and the material constants of *X*-axis-oriented Ta_2O_5 were used. The simulated values of effective electromechanical coupling factor (K^2_{eff}) for Ta_2O_5/Pt/Si and Ta_2O_5/Si structures as a function of the normalized Ta_2O_5 film thickness are shown in **Fig. 4**. It was found that the Ta_2O_5/Pt/Si structure exhibits a larger K^2_{eff} than the Ta_2O_5/Si structure when h_t/λ is greater than 0.46.

Figure 5 shows simulated particle displacements in the longitudinal (L) and shear vertical (SV) directions for each structure. The particle displacement in the shear horizontal direction was almost zero for each structure (h_t/λ=0.46). The particle displacement in the SV direction was distributed throughout the Ta_2O_5 thin film because the particles were concentrated in the Pt intermediate layer. From the above results, a larger coupling factor can be expected by adding a Pt thin film as an intermediate layer.

5. Conclusions

An *X*-axis-oriented Ta_2O_5 thin film was deposited on Pt/Si substrate using an RF magnetron sputtering system. The orientation and BAW properties were evaluated, and high coupling due to the effect of the concentration of displaced SAW particles was investigated theoretically using high-density Pt.

From the XRD pattern obtained, the Pt/Si sample showed a peak that did not exist for the Si sample. There is a possibility that the Ta_2O_5 crystal thin film that senses the lattice plane of Pt grows. From the pole figure plots, we determined that λ-Ta_2O_5 without piezoelectricity was grew. Therefore, the electromechanical coupling factor obtained from the HBAR response of this Pt-sensitive sample was smaller than that of the Pt-insensitive sample.

From FEM simulation, it is considered that the effective electromechanical coupling factor was increased by adding the Pt intermediate layer because the displaced SAW particles were distributed throughout the Ta_2O_5 thin film.

Acknowledgements

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