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Substrate temperature dependence of BAW propagation properties on (K,Na)NbO3 films deposited by RF sputtering

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1. Introduction

Acoustic wave devices, such as bulk acoustic wave (BAW) and surface acoustic wave (SAW) filters, are a crucial in wireless communication systems. Owing to the recent developments of next-generation communication systems, such as beyond 5G, the performance of these filters must be adequately improved. Accordingly, piezoelectric materials with large electromechanical coupling coefficients (k_t^2, K^2), low propagation losses, high phase velocities, and highly stable temperature properties need to be developed.

Aluminum nitride (AlN) films are used as piezoelectric films in BAW filters because of their high phase velocity and low propagation loss. Single crystals of $LiTaO_3$, $LiNbO_3$, and quartz were used in SAW filters. However, piezoelectric ceramics such as $Pb(Zr_xTi_{1-x})O_3$ (PZT) have greater piezoelectricity than the abovementioned piezoelectric materials. Consequently, they are commonly used in sensors and actuators. However, because they incur large acoustic losses owing to the domain walls, it is difficult to apply them to high-frequency devices such as SAW and BAW filters. In addition, because of concerns regarding the toxicity of the Pb contained in PZT, lead-free piezoelectric materials have been developed.

$(K,Na)NbO_3$ (KNN)-based piezoelectric materials are Pb-free and possess relatively high piezoelectricity. KNN thin films are mainly deposited using radio frequency (RF) magnetron sputtering.[1)] In a previous study, we evaluated the BAW propagation properties of KNN films formed on a Ti adhesion layer via RF magnetron sputtering, and obtained a k_t^2 value of 7.3 %.[2)]

In this study, the substrate temperature dependence of BAW propagation properties of a KNN film deposited using RF magnetron sputtering was evaluated.

2. Evaluation of BAW propagation properties

First, a ZnO thin film (thickness 25 nm) and Pt(111) thin film (thickness 200 nm) were formed as adhesion layer and bottom electrode, respectively, on a SiO_2/Si(100) substrate. Second, a KNN thin film (thickness t=2.0 μm) was formed on the Pt(111) thin film at a substrate temperature range of 400–740°C using an RF magnetron sputtering system with a ceramic target appropriately prepared such that the KNN thin film exhibited a composition ratio Na/(K+Na) of 0.65. This film was polycrystalline and had a pseudo-cubic perovskite structure with a preferential (001) orientation. Then, an Au thin film was vacuum-deposited on the surface of the KNN film as the top electrode, and a high-overtone bulk acoustic resonator (HBAR) with top electrode/piezoelectric thin film/bottom electrode/substrate was fabricated. The top electrode area of the HBAR was adjusted so that the input impedance was approximately 50 Ω at the longitudinal wave resonance frequency.

The conversion loss between the top and bottom electrodes was measured using a network analyzer. When a high-frequency electric field was applied to the electrodes, a bulk wave was excited, reflected by the bottom surface of the substrate, and converted into a voltage signal through the KNN film. The insertion loss was determined by the

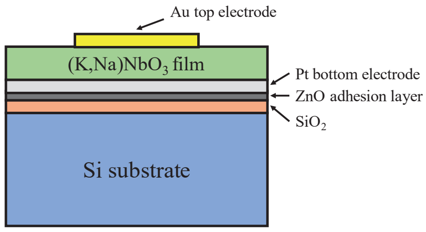

Fig. 1 Au/KNN/Pt/Si HBAR structure.

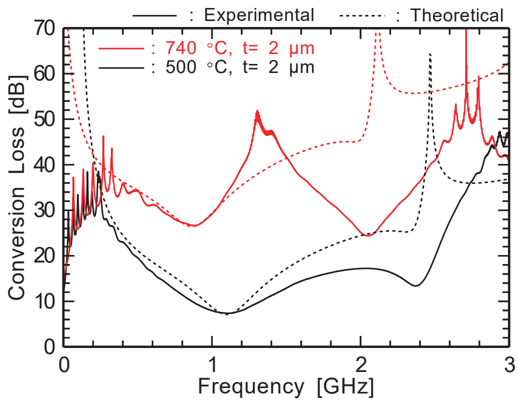

Fig. 2 Experimental and theoretical conversion losses of HBAR with a substrate temperature of 500°C and 740°C.

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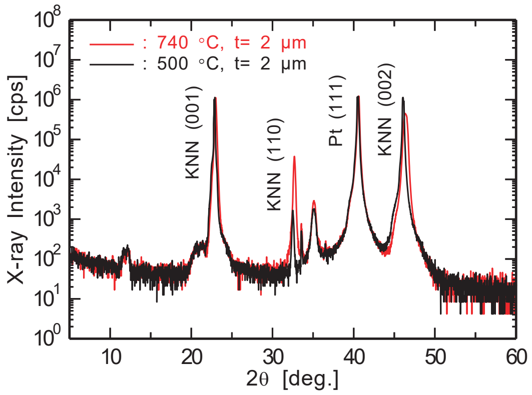

Fig. 3 2*θ*/*θ* XRD patterns of sample with KNN film at a substrate temperature of 500 °C and 740 °C.

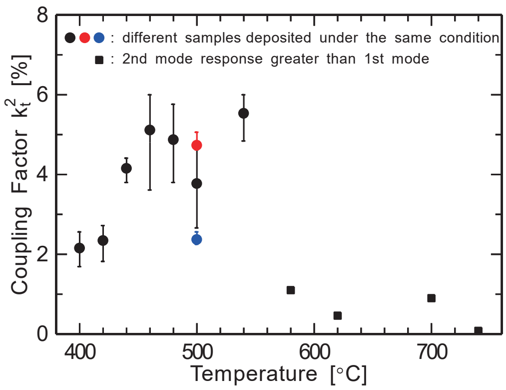

Fig. 4 Electromechanical coupling coefficient k_t^2 evaluated for HBAR.

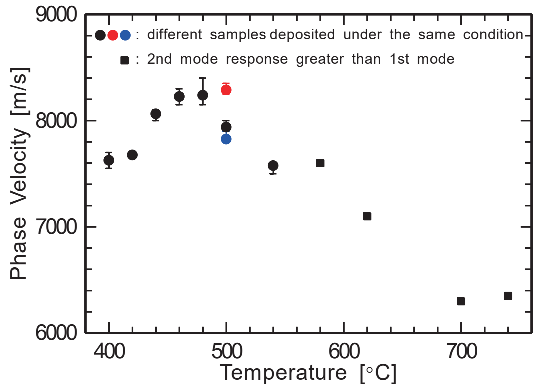

Fig. 5 Phase velocity evaluated for HBAR.

Fourier transform of the response in the time domain, and which was multiplied by 1/2 to obtain the conversion loss.

The electromechanical coupling coefficient k_t^2 and phase velocity were obtained by fitting the measured curve to the theoretical curve using the Mason equivalent circuit model. To evaluate the dispersion due to the measuring point, four points on each sample were considered. Subsequently, the average of values measured at these four points was used as the evaluated k_t^2.

3. Substrate temperature dependence of BAW propagation properties

Figure 2 shows examples of the HBAR conversion losses with a substrate temperature of 500°C and 740°C. The sample at 500°C exhibits greater 1st mode response of 1.1 GHz than 2nd mode response of 2.4 GHz. On the other hand, 2nd mode response is greater than 1st mode response on the sample at 740°C.

Figure 3 shows the X-ray diffraction (XRD) patterns of a KNN film at substrate temperatures of 500°C and 740°C. The XRD peaks of KNN(001), KNN(110), Pt(111), and KNN(002) were clearly observed. Focusing on KNN(110) peak, the XRD intensity of the sample at 740°C was greater than that of the sample at 500°C. Therefore, with an increase of substrate temperature at above 500°C, the poly-crystallization of the KNN film was promoted. In other words, different polarization axes were formed. There is a possibility that this difference in the crystalline structure affects the magnitude difference in 2nd mode response between the sample at 500°C and that at 740°C.

Figures 4 and **5** show the measured k_t^2 and phase velocity, respectively, as functions of the substrate temperature. The maximum k_t^2 value of 6.0 % was obtained at a substrate temperature of 460°C. It was observed that k_t^2 tends to increase with an increase in substrate temperature below 460°C.

On the other hand, k_t^2 value at substrate temperatures above 580°C were obtained by fitting the conversion loss where the 2nd mode response is greater than the 1st mode response, as described above.

4. Conclusion

In this study, the substrate temperature dependence of the BAW propagation properties of a KNN film deposited using RF magnetron sputtering was evaluated. We clarified that k_t^2 tends to increase with an increase in a substrate temperature below 460°C, while the poly-crystallization of the KNN film promoted with the increase of a substrate temperature at above 500°C.

In the future, we will investigate the optimization of the KNN deposition conditions to obtain a larger electromechanical coupling coefficient and attempt to fabricate a film bulk acoustic resonator (FBAR) using KNN films.

References

1) K. Shibata, *et al.*, Jpn. J. Appl. Phys. **50**, 041503 (2011).
2) K. Yoshizawa, *et al.*, Jpn. J. Appl. Phys. **61**, SG1077 (2022).