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Evaluation of electromechanical coupling coefficients of (K,Na)NbO_3 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 crucial in wireless communication systems. Therefore, there exists a need for piezoelectric materials with large electromechanical coupling coefficients (k_t^2, K^2), high quality factors (Q), high phase velocities, and highly stable temperature properties.

(K,Na)NbO_3 (KNN)-based piezoelectric materials are Pb-free and exhibit high piezoelectricity. KNN thin films are primarily deposited via radio frequency (RF) magnetron sputtering.[1)] In our previous study, high-overtone bulk acoustic resonators (HBARs) were fabricated using KNN films formed on a ZnO adhesion layer via RF magnetron sputtering, and the substrate temperature dependence of the BAW propagation properties of a KNN film obtained by the conversion-loss method was evaluated to optimize the KNN deposition conditions. We clarified that the optimum substrate temperature for obtaining a lager k_t^2 is approximately 500 °C.[2)]

In this study, film bulk acoustic resonators (FBARs) were fabricated using KNN thin films, and their resonance properties were evaluated to determine k_t^2. Moreover, the inactive piezoelectric layer in KNN films was investigated from the fitting results of conversion loss of HBARs.

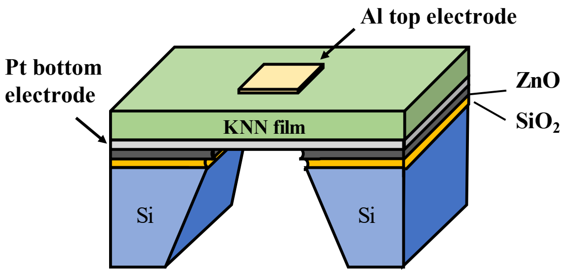

Fig. 1 Schematic diagram of the FBAR structure using oriented KNN films.

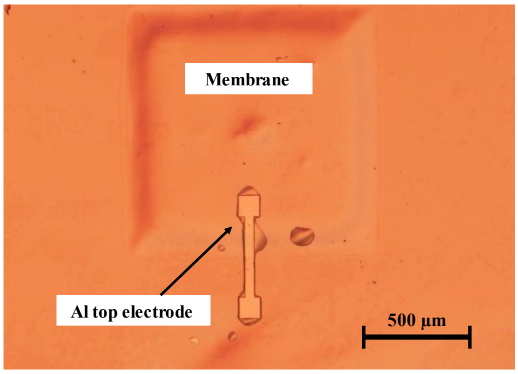

Fig. 2 Micrograph of the top view of the FBAR structure.

2. Evaluation of coupling coefficient using FBARs

First, a ZnO thin film (thickness = 25 nm) and a Pt(111) thin film (thickness = 200 nm) were formed as the adhesion layer and bottom electrode, respectively, on a SiO_2/Si(100)/SiO_2 substrate. Subsequently, 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. The film was polycrystalline and exhibited a pseudo-cubic perovskite structure with a preferential (001) orientation. Subsequently, lithography and lift-off processes using a negative photoresist were used for patterning to form a membrane with an area of 1.1 × 1.1 mm^2. The exposed KNN/Pt/ZnO/SiO_2/Si multilayer structure was etched via KOH-based wet etching, using a Ta_2O_5 thin film as the protective film. Finally, a 100 nm thick Al top electrode with an area of 0.1 × 0.1 mm^2 was formed on the KNN film.

Figures 1 and **2** show the FBAR structure using oriented KNN films and the micrograph of the top view of the FBAR sample at 500 °C. The frequency admittance was measured using a network analyzer, and k_t^2 was extracted by fitting the theoretical value calculated using Mason's equivalent circuit model.

Figure 3 shows examples of the experimental and theoretical admittances of the FBAR with a substrate temperature of 500 °C. The fundamental (1st) and 5th mode responses were observed at approximately 1.05 and 4.0 GHz on the sample at 500 °C. From the fitting results, a k_t^2 of 16.0% and a material Q factor (Q_m) of 8 were obtained. The theoretical result with Q_m = 100 is also shown in the figure to indicate the resonance and anti-resonance frequencies of the 1st mode response. An effective electromechanical coupling factor k_{eff}^2 of 20.1% was obtained from these frequencies.

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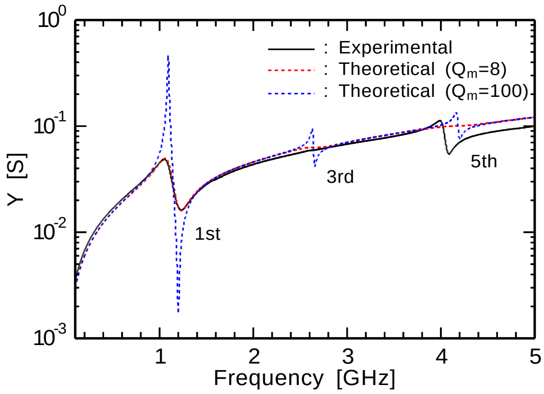

Fig. 3 Experimental and theoretical frequency characteristics of the admittance in KNN FBAR.

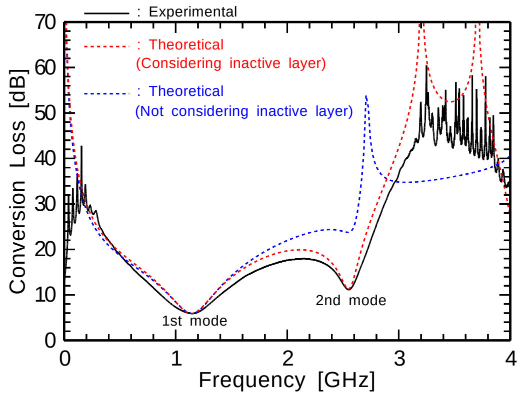

Fig. 5 Experimental and theoretical conversion loss in the KNN HBAR sample at a substrate temperature of 500 °C.

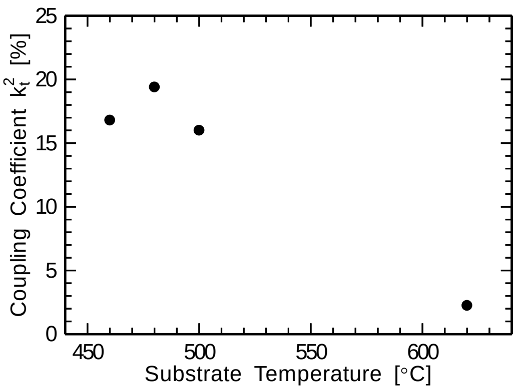

Fig. 4 Electromechanical coupling coefficient k_t^2 evaluated for KNN FBAR.

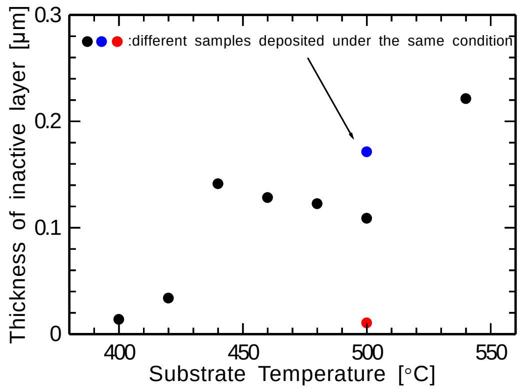

Fig. 6 Temperature dependence of the thickness of the inactive piezoelectric layer in oriented KNN films.

Figure 4 shows k_t^2 as a function of the substrate temperature. A similar temperature dependence was observed for the HBARs. The maximum k_t^2 value of 19.4% was obtained at a substrate temperature of 480 °C.

3. Inactive piezoelectric layer in KNN films

Figure 5 shows the experimental and theoretical conversion loss with and without the inactive piezoelectric layer in the KNN HBAR sample at a substrate temperature of 500 °C. A high fitting accuracy was obtained in the 2nd mode response at a substrate temperature range of 400–540 °C by considering the inactive piezoelectric layer.

Figure 6 shows the temperature dependence of the inactive piezoelectric layer thickness in the KNN films. Based on this result, it was determined that 1–10% of the inactive piezoelectric layer was formed in the oriented KNN films. Given the inactive piezoelectric layer, the k_t^2 value was evaluated to be 20.3% at a substrate temperature of 480 °C. Additionally, the 3rd mode response of the theoretical admittance shown in Fig. 3 is greater when the inactive piezoelectric layer was applied to the equivalent circuit.

4. Conclusion

In this study, the electromechanical coupling coefficients k_t^2 of KNN films deposited via RF magnetron sputtering were evaluated using FBAR structures. Moreover, the inactive piezoelectric layer in the KNN films was investigated based on the fitting results of the conversion loss of the HBARs. A maximum k_t^2 value of 19.4% was obtained at a substrate temperature of 480 °C, while the Q_m of oriented KNN films was approximately 10, which is insufficient for devices such as filters. In addition, we demonstrated the possibility of forming an inactive piezoelectric layer in oriented KNN films.

In the future, we aim to investigate the optimization of KNN fabrication conditions to obtain a larger electromechanical coupling coefficient and higher quality factors and attempt to fabricate FBAR using epitaxial KNN films.

References

1) K. Shibata, *et al.*, Jpn. J. Appl. Phys. **50**, 041503 (2011).
2) Y. Nakayama, *et al.,* Proc. USE, 3P3-6, (2023).