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Investigation of polarization switching behavior in epitaxial PZT films by using GHz ultrasonic excitation characteristics

GHz 帯超音波励振を用いたエピタキシャル PZT 薄膜の分極反転挙動観察

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1. Introduction

Single crystalline PZT has attracted interest for high Q resonator and tunable filters [1)]. However, bulk single crystalline PZT near MPB can not be grown, and therefore the most common approach to obtain single crystalline PZT is epitaxial growth technique. General epitaxial substrate: $SrTiO_3$ or MgO is difficult to etch away. Therefore, FBAR resonance- antiresonance method which is the most accurate method to obtain electromechanical coupling coefficient k_t in the GHz range cannot be used.

In this study, GHz intrinsic k_t value of single crystalline PZT films was extracted from HBAR (High-overtone bulk acoustic resonator) structure including substrate. Moreover, the polarization swiching behavior of random polarization layer (piezoelectric inactive layer) existing at initial stage of the growth was investigated using conversion loss curve of the resonator.

2. PZT film growth

(001) $Pb(Zr_{0.53}Ti_{0.47})O_3$ thin films near MPB with 2.8 μm or 4.4 μm were grown on (101)$SrRuO_3$/(001)Pt: total 100 nm /(001) MgO: 0.3 mm substrate or La doped $SrTiO_3$: 0.5 mm conductive substrate by using an RF magnetron sputtering with powder target [2)]. RF power, pressure, and substrate temperature were set to 100 W, 0.5 Pa, 600 ºC, respectively. Growth rate is approximately 200 nm/h.

3. k_t extraction in HBAR structure

First, impulse response of HBAR is obtained by an inverse Fourier transform of S_{11} measured by a network analyzer. As shown in Fig. 1 (a), acoustic waves excited from PZT film propagate in $SrTiO_3$ substrate, reflect at substrate bottom, and is detected again by PZT film. Energy conversion efficiency so-called conversion loss (CL) can be obtained by Fourier transform of first longitudinal wave echo.

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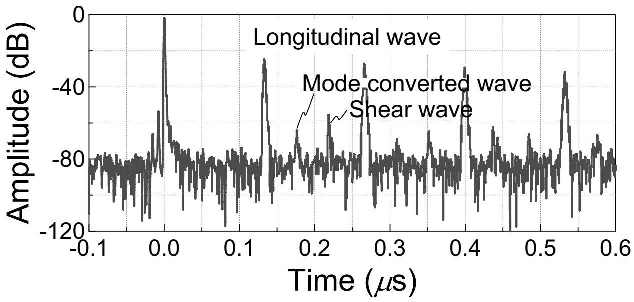

Fig. 1　Impulse response of the PZT/STO HBAR

The conversion loss includes 1)electromechanical coupling of the film, 2)mismatch between capacitive impedance of the film and 50 Ω measurement system, 3)transmission loss at boundary of each layer and substrate, 4)propagation and diffraction losses in the substrate. 2) and 3) can be simulated by Mason's equivalent circuit model including each layer. Therefore, k value can be extracted from the CL if 4) is negligibly small.

Film capacitance (dielectric constant) and parasitic inductance is determined from slope and electric resonance frequency of experimental admittance characteristics, and CL curves were simulated by using these values. Acoustic velocity and density of the PZT is set to 4522 m/s and 7605 kg/m^3 in the simulation, respectively.

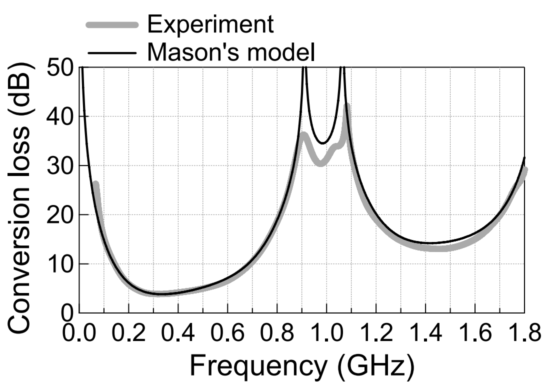

Fig. 2　Experimental and simulated conversion loss curves of the PZT/STO HBAR.

Fig. 2 shows the experimental and simulated CL curves. Simulated curve agreed well with the experimental curve, even though only k_t value is the adjustable parameter. In this case, k_t value of the PZT film was determined to be 0.42.

4. High temperature characteristics of the k_t

Next, in the same manner, we also investigated the high temperature characteristics of the k_t value of the epitaxial PZT film. Fig. 3 shows the k_t value determined at 30 to 550 ºC. k_t value of the epitaxial PZT film is highest compared with that of other high temperature piezoelectric films in our laboratory [3, 4]. High k_t were observed even above Curie temperature of bulk PZT, probably due to the epitaxial strain in the film.

5. Polarization swiching behavior of random polarization layer at PZT/SRO boundary

Figure 4 shows the experimental and simulated CL curves of PZT/SRO/Pt/MgO HBAR. 2nd-order thickness extensional mode excitation observed at 1.2 GHz in experimental CL indicates the existence of piezoelectric inactive layer at initial stage of PZT growth. Simulated curve in which the inactive layer is taken into account showed good agreement in detail with the experimental curve. k_t value is determined to be 0.395.

Next, 130 kV/cm was applied to the film to polarize the inactive layer. As a result, fundamental mode was enhanced and 2nd order mode was suppressed. In contrast to the previous result, simulated curve excluding the inactive layer agreed well with the experimental curve. k_t value increased to 0.42 after the polarization treatment. This result shows that high DC electric filed induces the polarization switching of the inactive layer.

6. Conclusion

k_t value of epitaxial PZT films were measured using $PZT/SrTiO_3$ HBAR, without removing substrate. As a result, k_t value was determined to be 0.42. High k_t were observed even at 600 ºC. Polarization switching behavior of random polarization layer at $PZT/SrRuO_3$ boundary was investigated using conversion loss curve of the resonator. The result showed that random polarization layer vanishes after the polarization treatment. This method is an effective tool to investigate polarization state and k_t value in the single crystalline PZT films. In situ polarization switching behavior under the bias DC electric field will be presented on the day of the symposium.

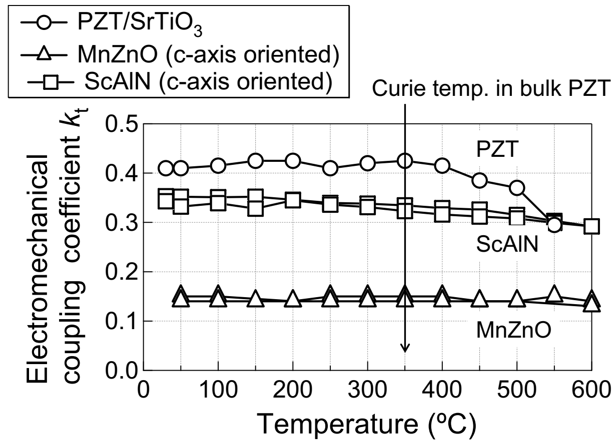

Fig. 3 Comparison of high temperature characteristics of the k_t value of the (001) $PZT/SrTiO_3$, (0001) ScAlN film, and (0001) MnZnO film.

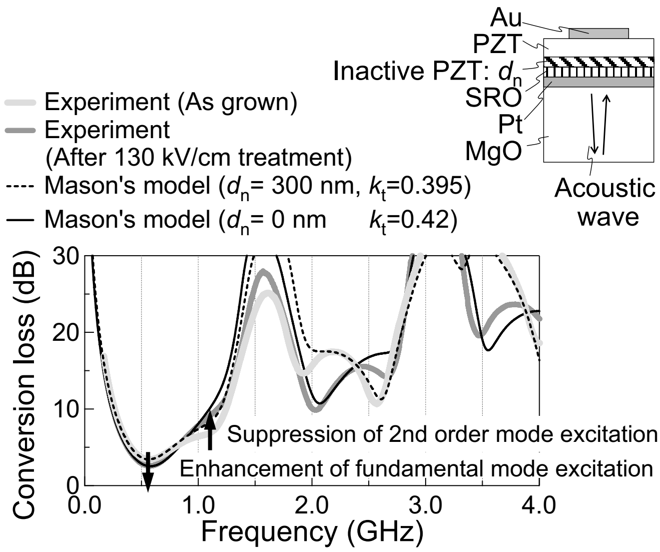

Fig. 4 Experimental and simulated conversion loss curves of the PZT/SRO/Pt/MgO HBAR. d_n is the thickness of the piezoelectric inactive PZT layer considered in the simulation model.

References

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