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Second overtone mode polarization inverted HBAR consisting of (001)/(00-1) $PbTiO_3$ epitaxial thin films

(001)/(00-1) $PbTiO_3$ エピタキシャル薄膜を用いた
二次モード複合共振子

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1. Introduction

Tunable bulk acoustic wave (BAW) resonator filter have attracted attention in recent years due to their potential application to microwave communications. For example, high tunability of 4.4 % with electromechanical coupling coefficient of 10 % was reported in $BiFeO_3$-$BaTiO_3$ film resonators[1]. On the other hand, the harmonic mode resonation in polarization inverted multilayer provides one possible way of realizing large tenability. Usual polarization unidirectional single layer resonator operates at fundamental (first) mode whereas the resonator consisting of double layer with opposite polarization operates at second harmonic mode. Polarization inverted ferroelectric thin mulitlayer structure make it possible to achieve two-way switching electrically between the harmonic mode operations. However, experimental studies of these structures have not been reported except paraelectric $BaSrTiO_3$ mutilayers reported by Vorobiev [2].

In this study, we experimentally demonstrated second harmonic thickness mode excitation in (001)/(00-1) polarization inverted $PbTiO_3$ film resonator structures.

2. Polarization inverted $PbTiO_3$ growth

Figure 1 shows the fabrication procedure of (001)/(001) polarization inverted structure. $PbTiO_3$ epitaxial films were grown by RF magnetron sputtering with powder target. Double-side polished 3.73 wt % La doped conductive (001) $SrTiO_3$ was used for substrates. Substrate temperature was approximately 550 ºC in the growth. Au electrode was deposited on the first $PbTiO_3$ layer (310 nm) and 13 V (420 kV/cm) was applied to invert polarization direction of the layer. Next, second layer of $PbTiO_3$ (375 nm) was growth to obtain polarization inverted double layer structure.

3. k_t estimation and resonator characteristics

During the procedure as shown in **Fig. 1**, electromechanical coupling coefficient k_t of the first $PbTiO_3$ layer was measured using conversion loss of the high-overtone bulk acoustic resonator structure (HBAR: top electrode / piezoelectric thin film / conductive substrate structure). Longitudinal wave conversion loss was measured by a network analyzer (E5071C, Agilent technologies, 100 kHz–4.5 GHz). **Figure 2 (a) and (b)** shows experimental conversion loss curve measured before and after the polarization treatment, respectively. Also described are the theoretical curve simulated by Mason's equivalent circuit model including electrode layer and parasitic inductance. k_t of layers was estimated by comparing experimental curve with theoretical one [3].

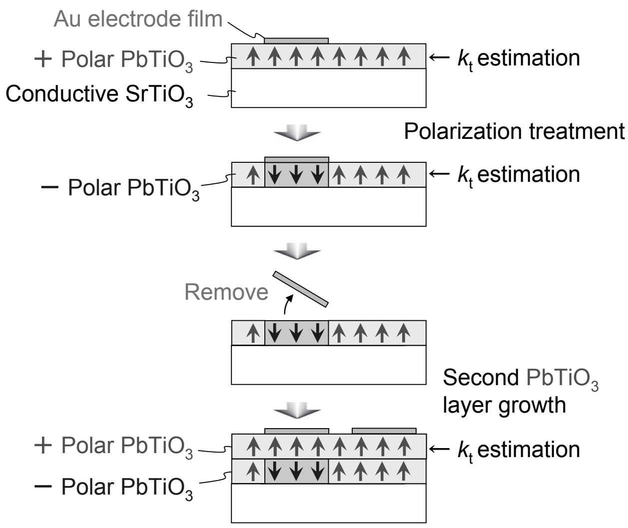

Fig.1 Fabrication procedure of (001)/(00-1) polarization inverted $PbTiO_3$ epitaxial film structure.

k_t value before and after the polarization treatment was estimated to be 0.53 and 0.44, respectively. Polarization directions (sign) of samples were determined by a press test [3]. **Fig. 3 (a) and (b)** shows the piezoelectric responses of $PbTiO_3$ films before and after the polarization treatment. Negative charge appeared in the film before the polarization treatment, when the compressive stress was applied. In contrast, positive charge appeared in the film after the polarization treatment. These results show that polarization direction of after the polarization treatment was inverted to before that, as expected.

After the second layer growth, the conversion loss was measured at the region where the polarization treatment was performed at first layer and where that was not performed. As shown in **Fig. 4 (a)**, fundamental thickness extensional mode resonance was observed at 1.3 GHz in the region where polarization direction of the first and second layer is same. In contrast, second mode resonance excitation was clearly observed at 3.6 GHz and fundamental mode resonance at 1.2 GHz was suppressed in the region where polarization direction of the first and second layer is opposite. Experimental curve shows good agreement with theoretical curve simulated by Mason's model considering polarization inverted structure [5].

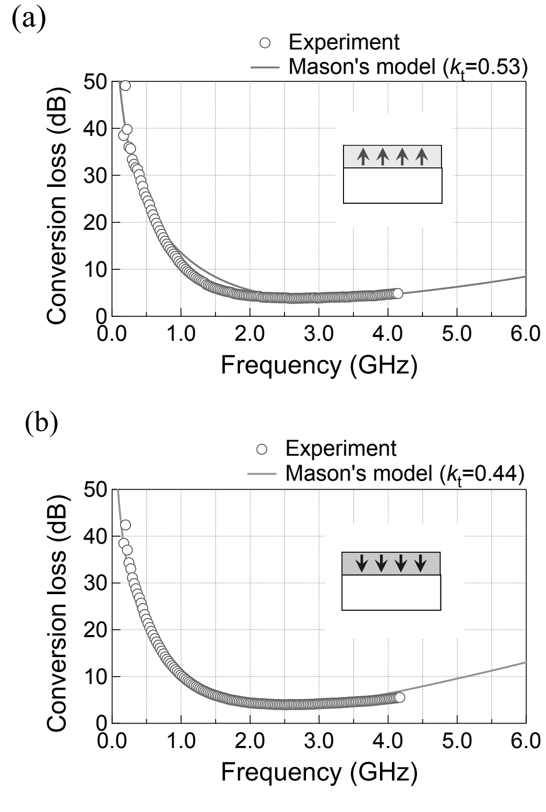

Fig. 2 Experimental conversion loss curve of (a) (001) $PbTiO_3/SrTiO_3$ HBAR (before the polarization treatment) and (b) (00-1) $PbTiO_3/SrTiO_3$ HBAR (after the polarization treatment), respectively. Also described are the theoretical curve simulated by Mason's model including electrode layer and parasitic inductance.

4. Conclusion

(001)/(00-1) polarization inverted $PbTiO_3$ epitaxial film resonator was fabricated. Second harmonic mode excitation with suppression of fundamental mode excitation was obtained. Electrically harmonic mode switchable resonator filter is expected in the future by inserting conductive $SrTiO_3$ layer between the polarization inverted double layers.

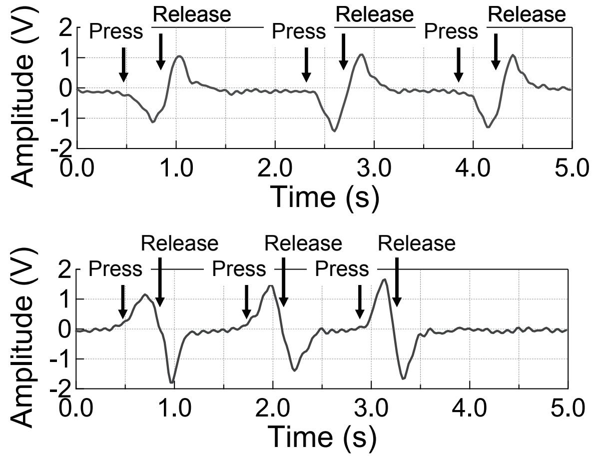

Fig. 3 Piezoelectric responses of first $PbTiO_3$ layer when compressive stress were applied (a) before and (b) after the polarization treatment

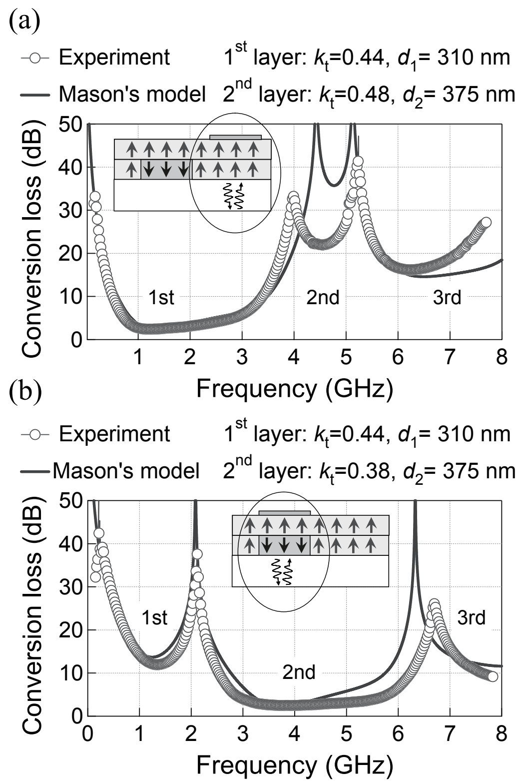

Fig. 5 Experimental conversion loss curve of (a) (001)/(001) $PbTiO_3/SrTiO_3$ HBAR (in the region where polarization direction of the first and second layer is same) and (b) (001)/(00-1) $PbTiO_3/SrTiO_3$ HBAR (in the region where polarization direction of the first and second layer is opposite), respectively..

References

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