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Mechanical Q factor dependence on Zr / Ti ratio of sputter-grown PZT epitaxial thin films

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1. Introduction

$Pb(Zr_xTi_{1-x})O_3$ (PZT) bulk ceramics are widely used for ultrasonic transducers and actuators because of their high piezoelectricity. On the other hand, PZT single crystalline thin films are attractive for GHz band thin-film resonator applications because of their expected higher mechanical Q factor (Q_m) than polycrystalline films. However, there are few reports on the Q_m of PZT single crystal thin film resonators.

Our group previously proposed a method to evaluate Q_m of the piezoelectric film without removing the substrate.[1] This method can determine Q_m of piezoelectric thin films grown on the substrates with a difficulty of etching, such as $SrTiO_3$.

In this study, Q_m of sputter-grown PZT epitaxial films grown on La-$SrTiO_3$ substrates was measured by using this method. The dependence of Q_m of $Pb(Zr_xTi_{1-x})O_3$ films on Zr / Ti ratio was investigated.

2. Principle of evaluating Q_m of the thin film with HBAR structure

Q_m of the entire HBAR (Q_{entire}) is affected by two factors: Q_m of the substrate (Q_{sub}) and Q_m of the thin film (Q_{piezo}). Since the mass of the film layer is much smaller than the mass of the substrate in the typical HBAR, Q_{entire} is nearly equal to the Q_{sub}. Nevertheless, Q_{piezo} has a more significant influence on Q_{entire} especially near the thickness resonant frequency of the thin film.

When Q_{piezo} is lower than Q_{sub}, the acoustic damping of the piezoelectric thin film results in the decrease of overall Q_{entire} in the vicinity of the resonant frequency of the thin films. The decrease in Q_{entire} near the resonant frequency of the thin film is determined by the ratio of Q_{sub} to Q_{piezo}. Therefore, Q_{piezo} can be estimated by using Q_{sub} as a reference.

3. Extraction of mechanical Q factor of PZT

Epitaxial (001) $Pb(Zr_xTi_{1-x})O_3$ films with different Zr / Ti ratio (x=0, 0.2, 0.4, 0.5, 0.6) were grown on conductive (100) La-$SrTiO_3$ single crystal substrate by RF magnetron sputtering. Ten mol% PbO rich PZT powder sputtering target is used to maintain the stoichiometry of PZT films.[2]

The real part of impedance (Z_{real}) was measured by a network analyzer (E5071C, Keysight Technologies) with various top electrode areas. Q_{entire} was acquired from multiple resonance peaks in the Z_{real}. Q_{piezo} was extracted by fitting the theoretical Q_{entire} to the experimental Q_{entire} in the vicinity of the resonant frequency of the films. Theoretical Q_{entire} was simulated by using Mason's equivalent circuit model.

Figure 1 shows the typical Q_{entire} of $Pb(Zr_xTi_{1-x})O_3$ / La-$SrTiO_3$ HBAR structure when x = 0. In this case, Q_m of the $PbTiO_3$ films was estimated to be 380.

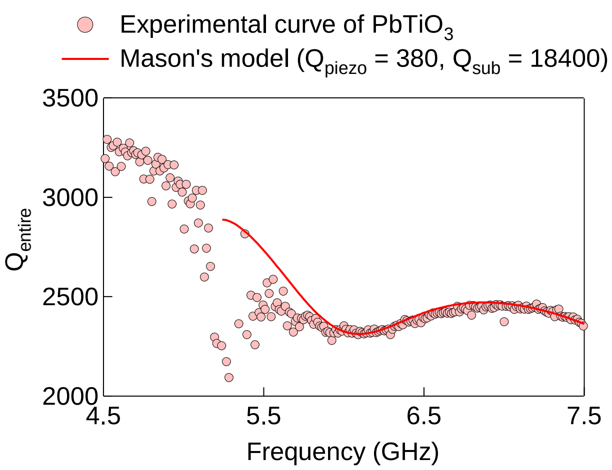

Fig. 1 Q_m factor of $PbTiO_3$ / La-$SrTiO_3$ HBAR structure and Q_m of $PbTiO_3$ thin film

4. Results and discussions

The relationship between Q_m of $Pb(Zr_xTi_{1-x})O_3$ films and Zr concentration is shown in **Fig. 2**. In this Q_m measurement method, the evaluated Q_{piezo} has an electrode area dependence.[3] The electrode area dependence of Q_m of $Pb(Zr_xTi_{1-x})O_3$, as shown in **Fig. 3,** should be caused by the leakage of acoustic waves in the lateral direction as surface acoustic waves. In this measurement, the highest value among

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the extracted Q_m is assumed to be the most accurate value owing to the minimum lateral acoustic wave leakage effect. As shown in Fig. 2, Q_m of $Pb(Zr_xTi_{1-x})O_3$ films decreases with increasing Zr concentration. Therefore, $PbTiO_3$ film is expected to possess the highest Q_m. In addition, we previously found that $PbTiO_3$ films exhibit the highest k_t^2 for sputter-grown PZT epitaxial thin films.[4] the product of k_t^2 and Q ($k_t^2 \cdot Q$), known as the figure of merit (FoM) of BAW resonator, indicates that $PbTiO_3$ film is the most suitable for resonator applications among the PZT material (**Fig. 4**).

According to a previous report of our group, sputter-grown $Pb(Zr_xTi_{1-x})O_3$ thin films with all Zr concentrations show the tetragonal structure and do not have morphotropic phase boundary (MPB), which is identified around x = 0.53 in bulk PZT.[4] However, a characteristically high Q_m of 400 was observed around MPB (x = 0.5).

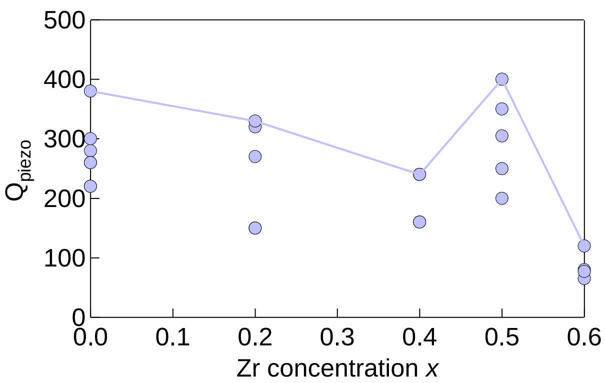

Fig. 2 The relationship between Q_m of $Pb(Zr_xTi_{1-x})O_3$ films and Zr concentration

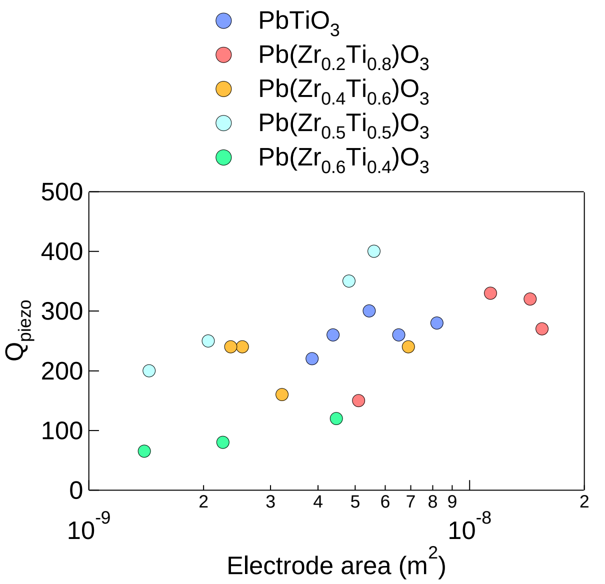

Fig. 3 The relationship between Q_m of $Pb(Zr_xTi_{1-x})O_3$ films and electrode area

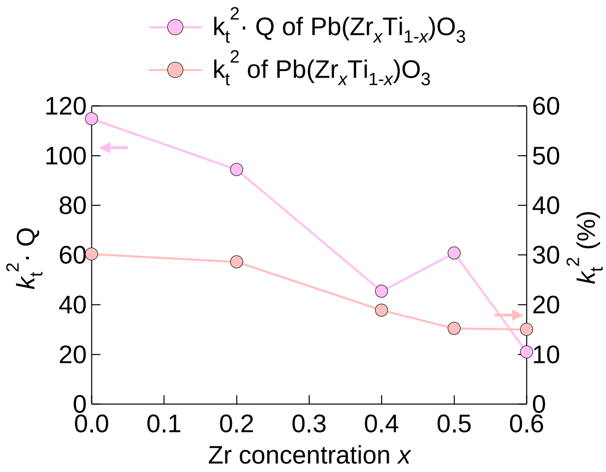

Fig. 4 $k_t^2 \cdot Q$ and k_t^2 of $Pb(Zr_xTi_{1-x})O_3$ films as a function of Zr concentration x

5. Conclusion

Q_m of sputter-grown $Pb(Zr_xTi_{1-x})O_3$ epitaxial thin films were evaluated at various Zr concentration (x = 0, 0.2, 0.4, 0.5, 0.6). The results show that Q_m of $Pb(Zr_xTi_{1-x})O_3$ films decreases with increasing Zr concentration. When x = 0, Q_m of $PbTiO_3$ thin film exhibit 380, and $k_t^2 \cdot Q$ exceeds 100. Therefore, $PbTiO_3$ epitaxial thin films are potential candidates for filter applications. On the other hand, a characteristically high Q_m of 400 was observed at x = 0.5, which is near the MPB of bulk PZT.

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References

1. S. Kinoshita and T. Yanagitani, Proc. IEEE Ultrason. Symp. 299 (2019).
2. K. Iijima, Y. Tomita, R. Takayama, and I. Ueda, J. Appl. Phys. **60** (1) 361 (1986).
3. N. Iwata, S. Kinoshita, and T. Yanagitani, Proc. IEEE Ultrason. Symp. 2095 (2020).
4. R. Noda, T. Shimidzu, K. Wasa, and T. Yanagitani, Proc. IEEE Ultrason. Symp. 13 (2019).