Piezoelectric Boundary Acoustic Wave in Cu electrode/ Rotated YX-LiNbO₃ Substrate Structure with Partially Covered SiO₂ Layer

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1. Introduction

It is known that for practical devices the temperature coefficient of frequency (TCF) is an important factor. Usually zero TCF is most preferred. Substrate material LiNbO3 or LiTaO3 has the negative TCF, while SiO₂ possesses positive TCF, it is possible to realize zero TCF device with SiO_2 over the substrate (shown in Fig. 1). Nakai and coworkers theoretically and experimentally discussed about the SiO₂ overlay shape (convex or concave or flat) influence on the Rayleigh SAW propagation characteristics, such as TCF, reflection coefficient, electromechanical coupling factor [1]. Yet, to the authors knowledge, there is no report on TCF of the SiO₂ slotted structure or topped structure. In this paper, we discuss about the SiO_2 influence allocation on the propagation characteristics of piezoelectric boundary acoustic wave (PBAW).

2. Simulation and Analysis

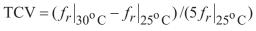
1. Simulation Steps:

The simulation is carried out for two kinds of SiO₂ allocation structures, slotted and topped as shown in Fig. 2 (a) and (b), where the YX-LN substrate is of semi-infinite. For metal grating materials, Cu grating is assumed. Cu thickness $h_{\rm m}$ is fixed at 0.2p [2]. In ref [2], where the structure is with semi-infinite SiO_2 overlay as shown in Fig. 1, numerical results showed that the temperature coefficient of velocity (TCV) of the PBAW resonance frequency could be $-2.88 \text{ ppm/}^{\circ}\text{C}$. In the following, the finite SiO2 with different allocation will be examined, especially its influence on the temperature coefficient. By changing the thickness of SiO₂ (represented by h_a and h_b in Fig.1, respectively), how the TCV of the PBAW would change.

Using the software – SYNCO, we calculated $\hat{Y}(\omega)$ of an infinitely long metal IDT of the structure as a function of the relative frequency $fp/V_{\rm B}$ ($V_{\rm B} = 4,752$ m/s is the fast-shear BAW velocity in LN). From the susceptance curve, we can get the resonance and anti-resonance frequency of certain modes ($f_{\rm r}$ and $f_{\rm a}$).

Then, we calculated relative admittance for various SiO_2 thickness to help distinguish the modes. The electro-mechanical coupling factor of one certain mode can be evaluated by the difference

of f_r and f_a . In addition, TCV of PBAW resonance frequency is estimated by



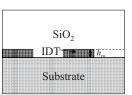
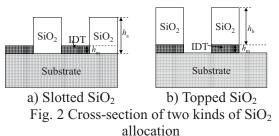


Fig. 1 Cross-section of SiO₂ semi-infinite overlay structure.



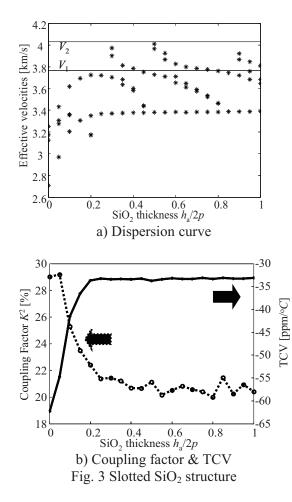
2. Simulation Results and Analysis

Fig. 3(a) shows the change in the effective velocities $(V_r=2f_rp, V_a=2f_ap)$ with the SiO₂ thickness for the slotted SiO₂ structure with the Cu grating, where V_2 (=4,031m/s) represents the slow shear bulk acoustic wave velocity in LN. V_1 (=3,766 m/s) is for the shear bulk acoustic wave velocity in SiO₂, which determines whether the acoustic wave is leaky or not; when $V < V_2$, it is non-leaky. Otherwise, it is leaky. We can see the coupling between different modes, which makes it quite difficult to distinguish the modes. However, it is quite clear that there is one straight branch which keeps constant and approaches to 3.4 km/s. Comparing this value with ref. [3], this should be the SH-type PBAW resonance frequency effective velocity. With the aid of RLC-model, we get the coupling factor K^2 curve shown in **Fig. 3(b)**, together with the TCV. The coupling factor decreases with the increase in SiO_2 thickness. In Fig. 3(b), when SiO_2 thickness is over 1p, K^2 tends to be maintaining constant though with some small fluctuations (within 2%). These fluctuations might be due to the mode-coupling as shown in Fig. 3(a). The PBAW coupling factor of 20% can be realized in this structure. Also, TCV tends to be constant around $-33 \text{ ppm/}^{\circ}\text{C}$.

For comparison, the same analyzing method is applied to the topped structure. Results are shown in **Fig. 4**, where (a) is the effective velocities; (b) is the K^2 and TCV curves. In (a), square and triangle modes are the higher modes, while circle mode is the mode of interest with non-leaky nature and relatively strong coupling. K^2 increases first and then decreases monotonically with the SiO₂ thickness, with its maximum value around 29.6%, at SiO₂ thickness 0.1*p*. When SiO₂ is over 1*p*, K^2 is less than 12%. This reflects that the mode is the resonance mode in the SiO₂ pillar, which can be further confirmed by the TCV result.

In **Fig. 4(b)**, TCV is improved gradually with the SiO₂, from -80 to +2 ppm/°C, and zero TCV can be realized with SiO₂ thickness 0.94*p*. However, there is no sign of convergence to some constant value; in other words, if we keep increasing the SiO₂ thickness, TCV will keep increasing. This indicates that this resonance mode is having the main energy concentrated within the SiO₂ pillar rather than the substrate surface. On the other hand, as shown in **Fig. 3** for the slotted SiO₂ structure, the PBAW would have its K^2 and TCV converging to some values and remain constant.

Table 1 compares the K^2 and TCV of two PBAW supported structure, with SiO₂ thickness fixed at 1*p*. This reveals that with overlay structure, better TCV can be achieved but K^2 will be sacrificed.



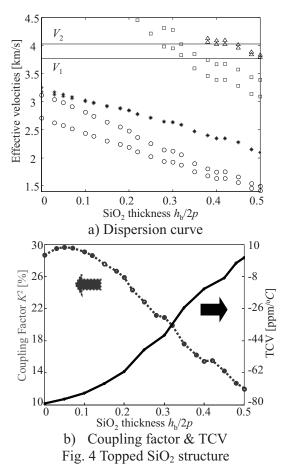


Table 1 PBAW supported structure comparison

	$K^{2}[\%]$	TCV [$ppm/^{\circ}C$]
Finite flat SiO ₂ overlay [3]	17.5	-1.85
Finite slotted SiO ₂	21	-33.1

3. Conclusion

In this paper, we discussed about the influence of the SiO₂ allocation on the acoustic wave propagation characteristics. In the simulation, Cu is used as metal grating, YX-LN as the substrate. Results show that in the slotted structure, there propagates the SH-type PBAW, which is similar to that of the SiO₂ overlay structure. If strong coupling is preferred, slotted SiO₂ structure is recommended; while good TCV is implemented using the finite flat SiO₂ overlay structure.

As for the topped structure, no PBAW wave is supported. Acoustic wave tends to have the energy concentrated in the SiO_2 , rather than the surface of the YX-LN.

References

- 1. Y. Nakai, *et al* : Proc. Ultrasonic Electronics Symp., (2008) 169~170.
- Y. Wang, *et al* : Proc. Frequency Control Symp., (2008) 773~777.
- 3. Y. Wang, *et al* : Proc. Ultrasonic Electronics Symp., (2008) 133~134.