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Theoretical analysis of Rayleigh SAW propagation characteristics on YbAlN films / high velocity substrates

YbAlN 層/高音速基板上を伝搬するレイリーSAW 特性解析

Masashi Suzuki† and Shoji Kakio (Univ. of Yamanashi)
鈴木 雅視†，垣尾 省司 (山梨大)

1. Introduction

SAW resonators with high frequency operation, wide bandwidth, high Q factor, and good temperature stability are required for applications to frequency filters in future mobile communications. However, standard SAW structures with IDTs / piezoelectric substrates cannot simultaneously achieve these performances. On the other hand, several researchers experimentally and theoretically demonstrated that LSAW, LLSAW, and high order mode RSAW resonators consisting of high piezoelectric material ($LiNbO_3$, $LiTaO_3$, and ScAlN) thin layer / high velocity substrate (Si, sapphire, quartz, and single crystalline diamond) enable high phase velocity, high coupling, low attenuation, and good temperature stability.

Since the increase of piezoelectricity in Sc doping AlN films was found by Akiyama *et al.*, the piezoelectricity and elasticity of other metal doped AlN films were studied experimentally and theoretically. The electromechanical coupling factors of MgZrAlN, YbAlN, and CrAlN film bulk acoustic wave resonators (FBARs) are higher than that of a pure AlN FBAR. Especially, the k_t^2 of YbAlN films exceed those of ScAlN films[1)]. Therefore, it is expected that SAWs on YbAlN layer / high velocity substrate have high coupling, as is the case of ScAlN film layered structure.

In this study, RSAW (0th, 1st, and 2nd modes) propagation characteristics on YbAlN films / high velocity Si, sapphire, wurtzite AlN, 6H-SiC, wurtzite BN, or diamond substrates were investigated theoretically. Moreover, the characteristics of IDTs / polarity inverted YbAlN film / substrate were simulated by FEM to investigate the effect of polarity inverted structure on the coupling factor.

2. RSAWs characteristics on YbAlN film /substrate

Phase velocities of 0th, 1st, and 2nd mode SAWs on (0°,0°,0°) $Yb_{0.33}Al_{0.67}N$ films / various substrates were analyzed by Farnell and Adler SAW propagation analysis method. K^2 was determined from $K^2 = 2*(v_f - v_m)/ v_f$ (v_f: phase velocity in an electrically free surface, v_m: phase velocity in a metallized surface). Elastic constants, piezoelectric constants, and density for $Yb_{0.33}Al_{0.67}N$ calculated by density function theory[1)] were used in this analysis.

masashis@yamanashi.ac.jp

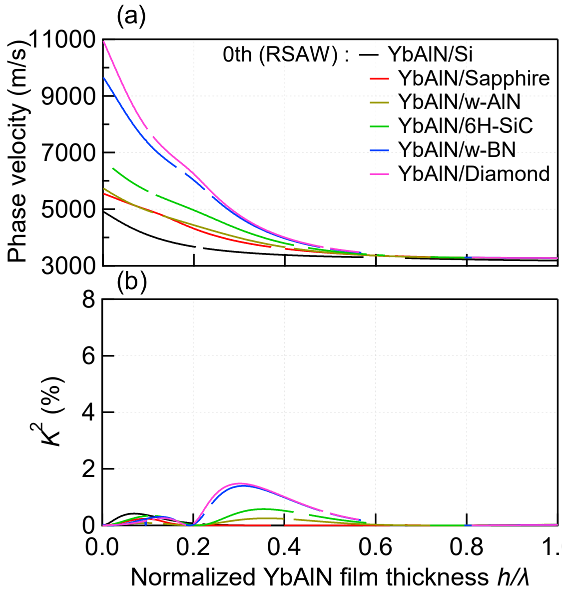

Fig. 1 (a) Phase velocities and (b) K^2 of 0th mode SAWs on (0°,0°,0°) $Yb_{0.33}Al_{0.67}N$ films / substrates.

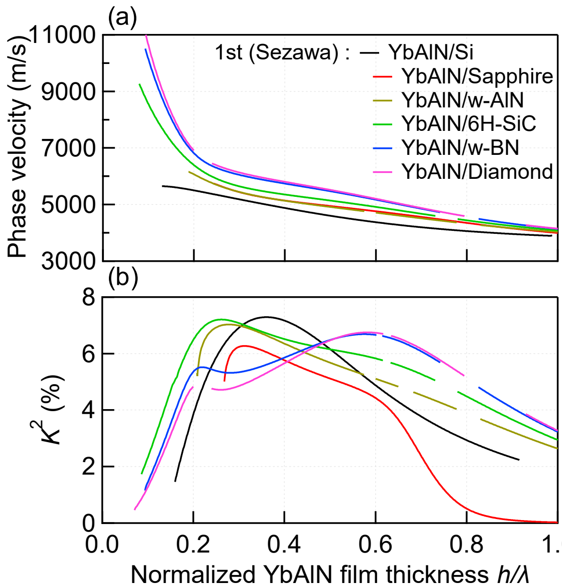

Fig. 2 (a) Phase velocities and (b) K^2 of 1st mode SAWs on (0°,0°,0°) $Yb_{0.33}Al_{0.67}N$ films / substrates.

We selected Si, sapphire, wurtzite AlN, 6H-SiC, wurtzite BN, or diamond as the substrate because these materials have higher RSAW phase velocity than that of $Yb_{0.33}Al_{0.67}N$.

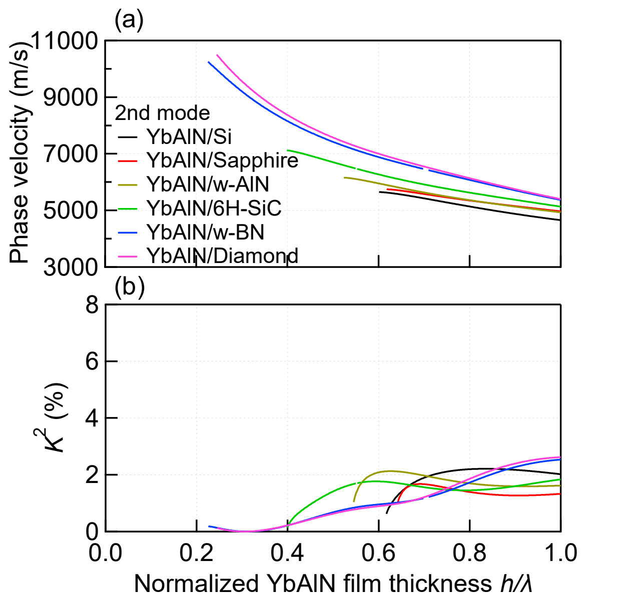

Fig. 3 (a) Phase velocities and (b) K^2 of 2nd mode SAWs on (0°,0°,0°) $Yb_{0.33}Al_{0.67}N$ films / substrates.

As shown in **Fig. 1(a)**, the phase velocities of 0th mode SAWs on YbAlN films / substrates decreased from the velocities of each substrate to approximately 3,300 m/s for the velocity of YbAlN with increasing the normalized YbAlN film thickness h/λ. The phase velocity of 1st mode and 2nd mode SAW also decreased with increasing h/λ, as shown in **Fig. 2(a) and Fig. 3(a)**. As shown in **Fig. 1(b)**, K^2 of 0th mode SAWs is less than 2% in all h/λ. As shown in **Fig. 3(b)**, maximum K^2 of 2nd mode SAWs is slightly larger than that of 0th mode SAWs. As shown in **Fig. 2(b)**, K^2 values of 1st mode SAWs were significantly higher than those of 0th and 2nd mode SAWs in all YbAlN film / substrate structure. The maximum K^2 values of the 1st mode SAWs were 6.3－7.3% for each YbAlN layered structure. These maximum values are higher than those of 1st mode SAW for $Sc_{0.4}Al_{0.6}N$ film layered structures.

3. FEM analysis for 1st-mode SAW on polarity inverted YbAlN film/substrate

A polarity inverted structure enhances the K^2 of 1st mode SAW on the ScAlN or AlN films / substrates[2]. We simulated the frequency characteristics of SAW resonators with Al IDTs / (0°,0°,0°) YbAlN layers/ (0°,180°,0°) YbAlN layers / substrates by FEM analysis (Femtet, murata software) shown in **Fig.4 (a)**. The total normalized YbAlN film thickness of 1st and 2nd YbAlN layer is fixed to be h/λ where the K^2 of 1st mode SAWs is the highest in mono layer YbAlN films / substrates. The k_{eff}^2 values of 1st mode SAWs on the layered structures were determined from the resonant and anti-resonant frequency obtained from **Fig. 4 (b)**. **Figure 5** shows the k_{eff}^2 values of 1st mode SAW on polarity inverted YbAlN film / each substrate as a function of 1st YbAlN layer thickness h_{1st}/λ. The k_{eff}^2

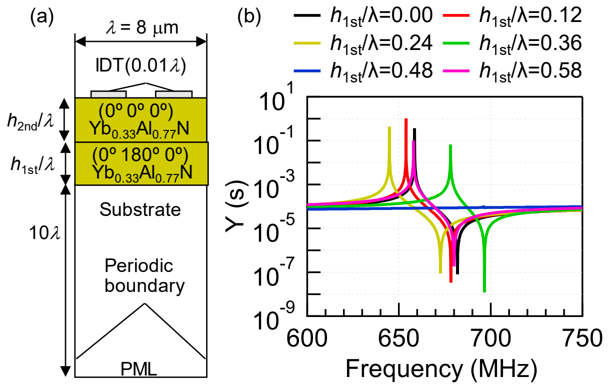

Fig. 4 (a) FEM model of Al IDT / Polarity inverted YbAlN film / substrate. (b) Admittance characteristics of 1st mode SAW resonance in IDT / polarity inverted YbAlN film / diamond substrate

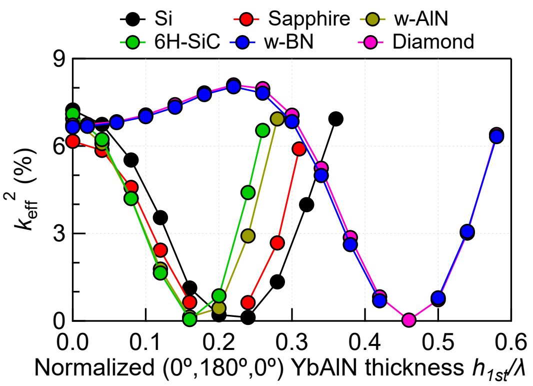

Fig. 5 k_{eff}^2 of 1st mode SAW on polarity inverted YbAlN films / each substrates as a function of h_{1st}/λ.

values in polarity inverted YbAlN film/ Si, sapphire, w-AlN, and 6H-SiC substrate were degraded with increasing h_{1st}/λ from 0 to 0.16-0.24. Above h_{1st}/λ = 0.16-0.24, the k_{eff}^2 are increased to the original k_{eff}^2 at $h_{1st}/\lambda = 0$. On the other hand, the k_{eff}^2 values in polarity inverted YbAlN film/ w-BN and diamond substrate were increased with increasing from h_{2nd}/λ from 0 to 0.22. The maximum k_{eff}^2 of approximately 8.0% were approximately 1.2 times higher than those of monolayer YbAlN film / w-BN or diamond substrates.

4. Conclusion

The propagation characteristics of 0th, 1st, and 2nd mode SAWs on YbAlN / high velocity Si, sapphire, w-AlN, 6H-SiC, w-BN, and diamond substrates were analyzed. We demonstrated that the all YbAlN layered structures had high K^2 in the 1st mode SAW. Moreover, the k_{eff}^2 of the 1st mode SAW was enhanced by using the layered structure with polarity inverted YbAlN film / BN or diamond substrate.

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References

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