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Enhancement of coupling factor K^2 in higher-mode RSAW on polarity inverted ScAlN films/high velocity AlN or BN substrates
分極反転 ScAlN 薄膜/高音速 AlN,BN 基板上を伝搬する
高次モード RSAW の結合係数 K^2 増幅

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1. Introduction

To develop next generation communication systems, high-performance surface acoustic wave (SAW) devices with a high frequency, a high electromechanical coupling factor (K^2), and a high Q factor are required. A SAW resonator with aluminum nitride (AlN) film/high phase velocity substrate structure can operate above 2 GHz and has a high Q factor. However, it is not appropriate for wideband filters because the low K^2 of approximately 1.2% in 1st mode Rayleigh SAW (RSAW) on AlN film/diamond substrate[1].

Recently, it was reported that scandium (Sc) doping in AlN films enhances the coupling factor. In the IDT/ScAlN film/diamond substrate structure, the maximum K^2 of approximately 5.5% in the 1st mode RSAW is approximately 4.6 times higher than that in the AlN film/diamond substrate structure[2]. Furthermore, the K^2 of 15.3% in the 1st mode RSAW on ScAlN films/IDT/polarity inverted ScAlN film/diamond substrate structure was approximately 2.8 times higher than that in IDT/ScAlN films/diamond substrate structure[3].

In this study, 0th-3rd mode SAW propagation characteristics on ScAlN film/high velocity AlN or boron nitride (BN) substrate structure were analyzed to find the optimal structure for high K^2 and high frequency. Moreover, we analyzed the characteristics of the 3rd mode RSAW propagating on the polarity inverted ScAlN film/high velocity BN substrate. The effect of the boundary position of the polarity inverted ScAlN film on the K^2 of the higher mode RSAW was also investigated by finite element method (FEM).

2. RSAW propagation on ScAlN films/AlN or BN substrate

The phase velocity and K^2 of RSAW on the (0º,0º,0º) ScAlN film/(0º,0º,0º) AlN or BN substrate structure were analyzed by Farnel and Adler's SAW propagation analysis. AlN (phase velocity ≈ 5,700 m/s) and BN (phase velocity ≈ 11,000 m/s) were used as the substrate because they have a higher phase velocity than ScAlN film. **Figure 1** shows the relationships between the K^2 of 0th, 1st, 2nd, and 3rd mode RSAWs and

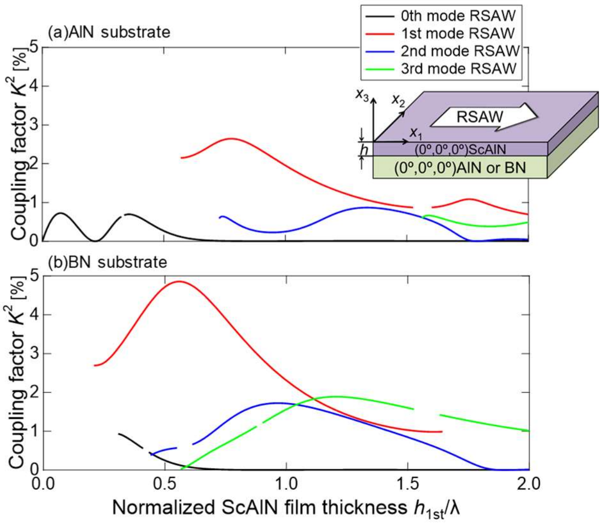

Fig. 1 The relationships between the K^2 and ScAlN film thickness h/λ on (a)ScAlN film/AlN substrate structure and (b)ScAlN film/BN substrate structure.

Table I The maximum K^2 and phase velocity for each mode RSAW on ScAlN film/AlN substrate structure and ScAlN film/BN substrate structure.

substrate	mode	h/λ	V [m/s]	K^2 [%]
AlN	0th	0.075	5519	0.73
	1st	0.778	5540	2.64
	2nd	1.335	5438	0.87
	3rd	1.589	6077	0.66
BN	0th	0.355	5534	0.87
	1st	0.559	6863	4.85
	2nd	0.965	6795	1.72
	3rd	1.205	7222	1.89

ScAlN film thickness h/λ. The maximum K^2 and phase velocity for each mode RSAW are shown in the **Table I**. The SAWs on the ScAlN film/BN substrate structure had a higher phase velocity and a higher K^2 than those on ScAlN film/AlN substrate structure, because their SAW particles were more concentrated in the ScAlN film. This is due to the fact that the phase velocity of a single crystal BN substrate is approximately twice as higher as that of a single crystal AlN substrate. In both structures, the highest K^2 were observed in the 1st mode RSAW. The maximum K^2 of the 2nd and 3rd mode RSAW were smaller than that of the 1st mode RSAW, and the phase velocity were almost the same as that of

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1st mode RSAW. However, in BN substrate, the maximum K^2 of the 2nd and 3rd mode RSAWs were higher than that of 0th mode RSAW.

Next, we investigated the effect of polarity inverted ScAlN film on the K^2 of 0th-3rd mode RSAW on ScAlN film/BN substrate. The phase velocity and K^2 of 0th-3rd mode RSAW on (0º,0º,0º) ScAlN film/(0º,180º,0º) ScAlN film/(0º,0º,0º) BN substrate structure was analyzed by Farnel and Adler's SAW propagation analysis. The total thickness of the two-layered ScAlN films was set to where the K^2 of each mode RSAW was maximum shown in **Table I**. **Figure 2** shows the relationship between the K^2 of each mode RSAW and 1st layer ScAlN film thickness h_{1st}/λ. The K^2 of each mode RSAW was enhanced by the polarity inverted ScAlN film structure, and the phase velocity did not significantly change. Moreover, the maximal K^2 in 2nd mode RSAW appeared at h_{1st}/λ=0.358. The maximal K^2 in 3rd mode RSAW also appeared at h_{1st}/λ=0.250 and 0.664. These enhancements of K^2 on polarity inverted ScAlN film structure were also confirmed in the polarity inverted ScAlN film/AlN substrate structure. In addition, K^2 of 0th, 1st, 2nd, and 3rd mode RSAWs are zero at h_{1st}/λ=0.135, 0.443, 0.844, and 1.099 respectively.

3. Finite Element Method Analysis

The frequency characteristics of admittance on IDT/one-layered ScAlN film/BN substrate and IDT/polarity inverted two-layered ScAlN films/BN substrate structure with maximum K^2 were analyzed by the FEM (Femtet, Murata software) shown in **Fig. 3**. The effective coupling factors (K_{eff}^2) of 3rd mode RSAW resonance were 1.84% in one-layered ScAlN film/BN substrate structure and 3.05% in polarity inverted two-layered ScAlN film/BN substrate structure. In addition, the color map in the **Fig. 2** shows the particle displacement of x_3 direction at resonant frequency in 3rd mode RSAW. The particle displacements were almost the same regardless of h_{1st}/λ. The particle displacement concentrated at depth/λ=0.194, 0.573, and 0.925. Setting the boundary of polarity inverted structure at the position, where the particle displacement is concentrated close at the film surface, can enhance the K^2 of 3rd mode RSAW effectively. If the boundary of polarity inverted structure is set at the all position where the particles are concentrated shown in color map in **Fig. 2**, K^2 of 3rd mode RSAW may be more enhanced. Therefore, we analyzed the frequency characteristics of admittance on Al IDT/polarity inverted four-layered ScAlN film/BN substrate structure. The K_{eff}^2 of 3.41% in the four-layered ScAlN films structure is about 1.85 times higher than that in one-layered ScAlN film structure, and about 1.12 times higher than that in two-layered structure. However, resonant frequency of four-layered ScAlN films structure is lower than that of one-layered and two-layered ScAlN films structure.

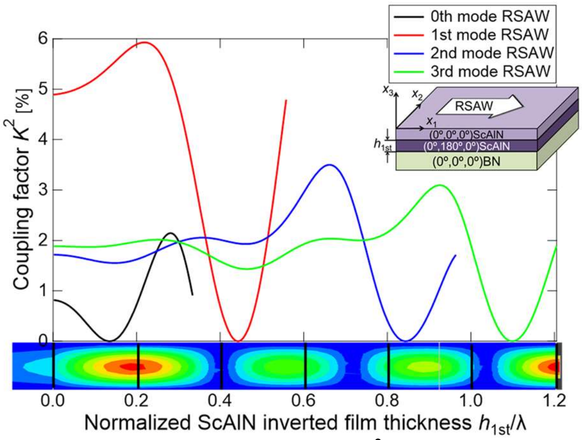

Fig. 2 The relationships between the K^2 and polarity inverted ScAlN film thickness h_{1st}/λ on (0º,0º,0º) ScAlN film /(0º,180º,0º) ScAlN film/(0º,0º,0º) BN substrate structure. Color map shows the particle displacement of x_3 direction at resonant frequency of 3rd mode RSAW with maximum K^2.

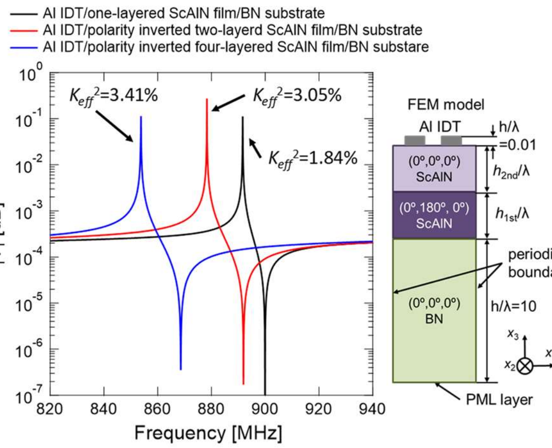

Fig. 3 The 3rd mode RSAW frequency characteristics of the admittance in Al IDT/one-layered ScAlN film/BN substrate structure, IDT/polarity inverted two-layered ScAlN films/BN substrate structure, and IDT/polarity inverted four-layered ScAlN films/BN substrate structure.

4. Conclusion

We analyzed the higher mode RSAW propagation characteristic and admittance characteristics of polarity inverted ScAlN film/AlN, BN substrate. In all modes, K^2 was higher in the ScAlN film/BN substrate structure than that in the ScAlN film/AlN substrate structure. The K^2 of the 3rd mode RSAW on polarity inverted two-layered ScAlN films/BN substrate structure was about 1.63 times higher than that of ScAlN film/BN substrate structure. The K_{eff}^2 was further enhanced by using polarity inverted four-layered ScAlN films structure.

References

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