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c-Axis Tilted or c-Axis Parallel ScAlN Films/Substrate SAW Devices with High Electromechanical Coupling

c 軸傾斜および平行配向 ScAlN 薄膜/基板構造における
弾性表面波の高い電気機械結合係数

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1. Introduction

SAW devices are widely used for frequency filters[1)] and microsensors[2)]. Electromechanical coupling coefficient K^2 in the substrate structure determines the bandwidth of SAW filters and the limitation of sensitivity in SAW sensors. In order to improve the performance of these SAW devices, high K^2 SAW substrate has been searched in many studies.

It is well known that the K^2 value depends on the acoustic and piezoelectric properties in the substrate material. Recently, the significant increase of piezoelectricity was found in the Sc heavily doped AlN film. The value of the extensional piezoelectric constant d_{33} in $Sc_{0.43}Al_{0.57}N$ film was increased five-fold as compared with that in pure AlN film. Hashimoto et al. calculated SAW properties of the ScAlN film on high-velocity materials such as SiC and diamond[1)]. High K^2 values of more than 5% were achieved in the second (Sezawa) mode.

The K^2 value also depends on crystalline anisotropy of the substrate structure. **Fig. 1** shows the relationship between the direction of electric field and the electromechanical coupling coefficients of bulk quasi-longitudinal wave k'_{33} and bulk quasi-shear wave k'_{35} for ScAlN[3)]. The k'_{33} value reaches maximum in the case of the correspondence between c-axis direction and the electric field direction. On the other hand, the k'_{35} value reaches maximum at the c-axis direction tilted to the electric field. These results indicate the piezoelectric constant e_{33} strongly contributes to these electromechanical coupling coefficients. Based on these anisotropies, we considered that c-axis tilted or c-axis parallel ScAlN film could enhance the K^2 value in the case of SAWs.

Wurtzite films such as AlN and ZnO generally tend to grow in c-axis normal orientation. Therefore, K^2 value in the c-axis tilted ScAlN/diamond structure has not been investigated. On the other hand, in previous study, we demonstrated that c-axis tilted and c-axis parallel ScAlN films were grown on silica grass substrate[3,4)].

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In this study, we theoretically investigated the K^2 values in the c-axis tilted or c-axis parallel ScAlN film on diamond substrate structure in SAWs. We then found the value of the c-axis tilt angle θ which maximizes K^2.

2. Calculation method

We analyzed the K^2 values of SAWs in c-axis tilted ScAlN/diamond structure as functions of normalized film thickness H/λ and c-axis tilt angle θ by using the Farnell and Adler's method[5)]. c-Axis tilt direction corresponds to the SAW propagation direction in the analysis. The K^2 values of the SAWs changes due to the configuration of the electrodes as shown in **Fig. 2**. Therefore, we calculated the K^2 values in these four configurations. Physical constants of $Sc_{0.4}Al_{0.6}N$ and diamond reported by Hashimoto et al.[1)] and Yamanouchi et al.[6)], respectively, were used in the analysis.

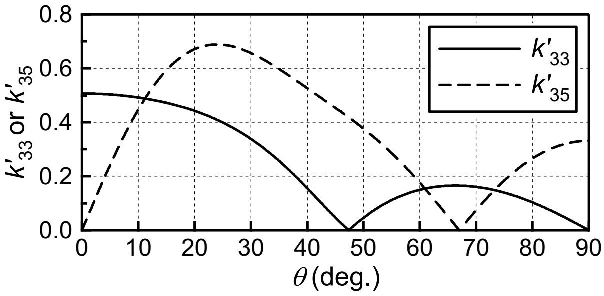

Fig. 1 Calculated electromechanical coupling coefficients of quasi-longitudinal wave k'_{33} and quasi-shear wave k'_{35} for ScAlN as a function of the angle θ between the c-axis and electric field direction[3)]. The physical constants of $Sc_{0.4}Al_{0.6}N$[1)] were used in the calculation.

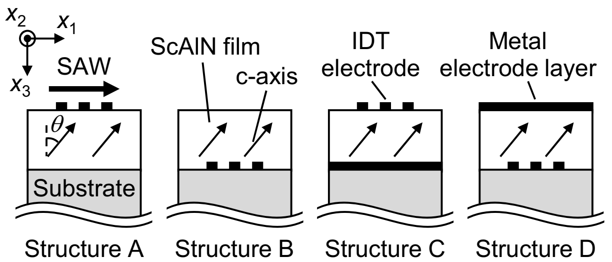

Fig. 2 Cross-sectional diagrams of the four types of film/substrate structures used in calculations.

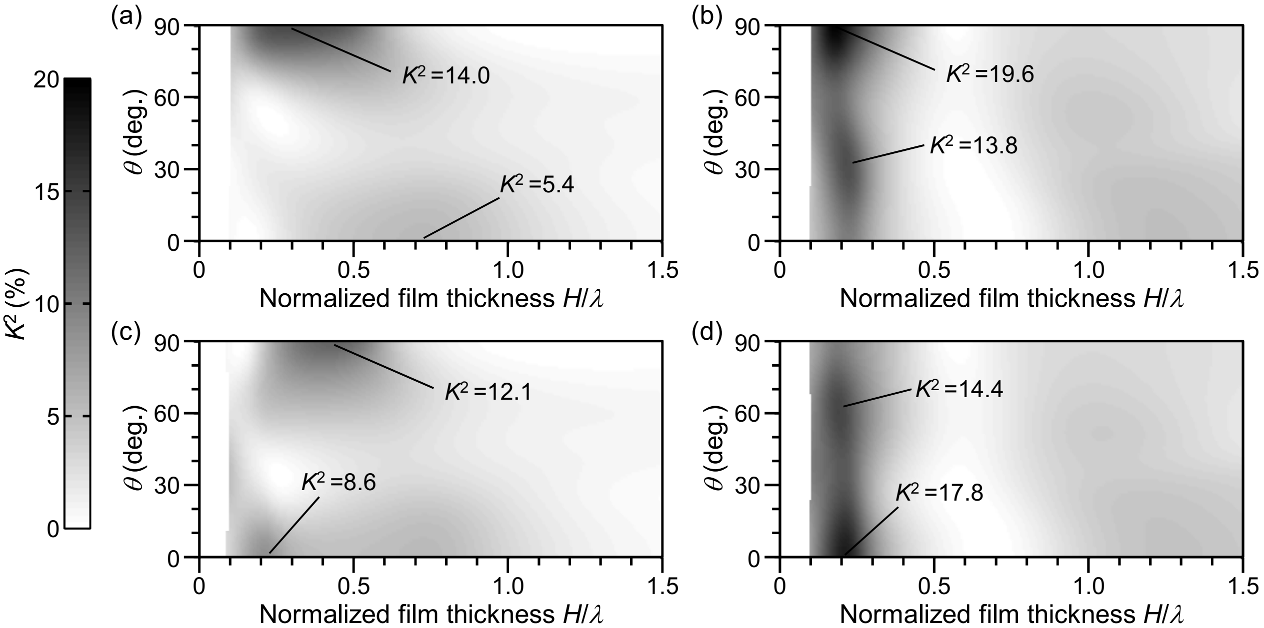

Fig. 3 Calculated electromechanical coupling coefficient K^2 of the second mode (Sezawa) SAW as a function of the c-axis tilt angle θ and normalized film thickness H/λ in (a) structure A, (b) structure B, (c) structure C, and (d) structure D.

3. Results and discussions

Fig. 3 shows contour plots of the calculated K^2 values of the second mode (Sezawa) SAW. Maximum K^2 value was found to be K^2 = 19.6% (phase velocity V = 9550 m/s) at H/λ = 0.18 and θ = 90º in structure B. θ of 90º means that the c-axis of ScAlN is parallel to the substrate plane. On the other hand, high K^2 value of 17.8% was found at θ = 0º in structure D. θ of 0º means the usual c-axis oriented film. The difference between these results is probably caused by the highest piezoelectric constant e_{33}. Because the electric field perpendicular to the substrate plane was enhanced by the metal over layer in structure D, highly piezoelectric effect was exhibited by the e_{33} at θ = 0º. In contrast, enhancement of the electric field parallel to the substrate plane in structure B resulted in the maximum K^2 value by the e_{33} at θ = 90º.

Although the high K^2 values were found in structure B and D, sample preparations of these structures are difficult because a film growth on IDT is required. On the other hand, sample preparations of structure A and C are not difficult. The K^2 value at H/λ = 0.29 and θ = 90º in structure A was relatively high (K^2 = 14.0%, V = 8660 m/s). This K^2 value in structure A consisting of c-axis parallel film (θ = 90º) was much higher than that of the usual c-axis oriented film (θ = 0º). **Fig. 4** shows the profile curves of K^2 as a function of H/λ at θ = 90º in structure A. The K^2 value of the second mode at H/λ = 0.29 was also higher than that of the other mode. As a result, the second mode SAW in c-axis parallel ScAlN/diamond structure is a promising candidate for SAW devices.

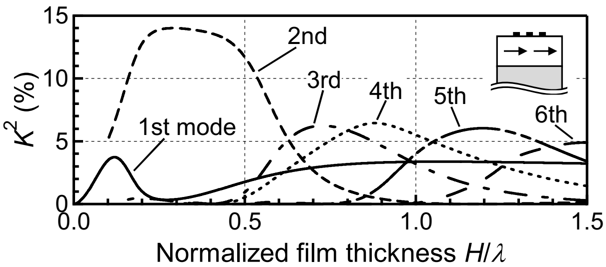

Fig. 4 Profile curves of K^2 as a function of H/λ in structure A consisting of c-axis parallel ScAlN film (θ = 90º).

4. Conclusions

In this study, the theoretically analyzed the K^2 value in the c-axis tilted ScAlN film on diamond substrate structure. In the result, the theoretical analysis showed that c-axis parallel ScAlN/IDT/diamond structure had a maximum K^2 value of 19.6% in second mode SAW. Experimental analyses of SAW devices consisting of c-axis parallel ScAlN film are expected.

References

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