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Effect of Sc concentration on quasi-shear mode electromechanical coupling k'_{15} in c-axis tilted ScAlN films

c 軸傾斜 $Sc_xAl_{1-x}N$ 薄膜(0<x<0.55)における擬似すべりモード電気機械結合係数

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1. Introduction

Shear mode AlN film resonators are suitable for liquid sensor and bio-sensor applications [1]. High (quasi-) shear mode electromechnical coupling k_{15} is required for the sensor applications. It is well-known that the k'_{15} of an AlN depends on the c-axis tilt angle [2]. The k'_{15} reaches maximum at c-axis tilted angle of around 30º [2].

ScAlN has been attracted as a potential piezoelectric material for BAW and SAW resonators. We reported the relationship between the extensional mode electromechnical coupling k_t^2 and Sc concentration in c-axis oriented ScAlN film [3]. The k_t^2 of the ScAlN film near the phase boundary was approximately twice of that of pure AlN single crystal [3]. For quasi-shear mode, c-axis tilted ScAlN films may possess significantly higher k'_{15} than that of pure AlN single crystal, as well as extensional mode.

In this study, c-axis tilted $Sc_xAl_{1-x}N$ (0<x<0.55) films were grown by an oblique angle sputtering deposition. The effect of Sc concentration on the c-axis tilted angle, the k'^2_{15}, and the quasi-shear wave velocity V'_{44} in c-axis tilted ScAlN film were estimated.

2. Growth of c-axis tilted ScAlN film

The ScAlN films with c-axis tilted angle of around 30º were grown by using the oblique angle sputtering deposition shown in **Fig. 1**. The incident angle of sputtered particles from the target affects the c-axis direction in the AlN film. Therefore, as shown in **Fig. 1**, the substrate angle to the target surface plane was adjusted to be 60º. Sc ingots were placed on the Al target to obtain the ScAlN films. The cathode RF power was set to be 200 W. The total gas pressure and N_2/Ar gas ratio were 0.75 Pa and 1/2, respectively. Al bottom electrode (120 nm)/silica glass (0.5 mm) was used as the substrate. Eleven ScAlN samples with 0–3.0 g of Sc ingot were prepared at 0.25 g intervals. One additional c-axis tilted ScAlN film was also prepared by using ScAl alloy target.

The Sc concentrations in the samples were estimated by an energy dispersive X-ray spectroscopy (EDX). Sc concentration in the samples was proportionally increased with increasing the amount of Sc ingots.

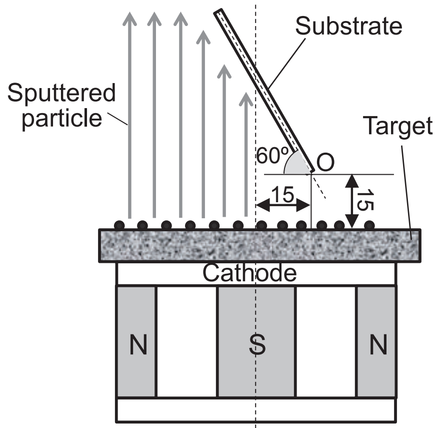

Fig. 1 Oblique angle sputtering deposition for c-axis tilted ScAlN film growth.

3. Crystalline orientation

The crystalline orientation of $Sc_xAl_{1-x}N$ (0< x <0.55) samples were estimated by an X-ray pole figure analysis. **Figs. 2** show the c-axis tilt angle as function of the distance from O point (the substrate edge near the target) in **Fig. 1**. As shown in **Fig. 2 (a)**, the c-axis tilt angles in the $Sc_xAl_{1-x}N$ samples with low Sc concentration (0<x<0.14) increased with the increase of the distance from O point. The c-axis tilt angles in the Sc concentration of 0.28<x<0.32 were nearly constant (**Fig. 2(b)**). In contrast, as show in **Fig. 2(c)**, the c-axis tilt angles in high Sc concentration (0.39<x<0.48) decreased with increasing of the distance from O point. On the other hand, the c-axis tilt angles in $Sc_{0.49}Al_{0.51}N$ films were lower than those of other ScAlN samples. This may be due to the phase transition from wurzite to cubic.

The ψ-scan FWHM of the all samples, indicating the dispersion of the c-axis tilt angle, were 6–10º.

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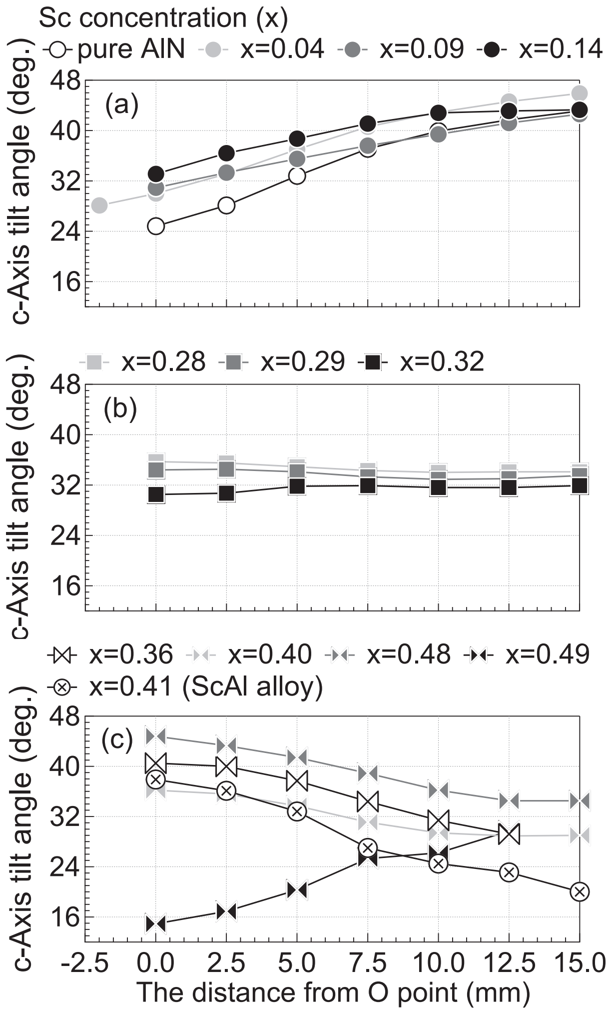

Fig. 2 c-axis tilt angle in $Sc_xAl_{1-x}N$ film samples (x=0–0.49) as function of the distance from O point. .

4. Shear mode k'_{15} and V'_{44}

High-overtone bulk acoustic wave resonators (HBARs) consisting of Au top electrode (100 nm)/c-axis tilted $Sc_xAl_{1-x}N$ film ($0<x<0.55$, c-axis tilt angle = 20–39º)/Al bottom electrode film/silica glass substrate were prepared. The k'^2_{15} and V'_{44} of the ScAlN films were determined by comparing the experimental and theoretical shear wave conversion loss (*CL*) curve of the resonators. The experimental shear wave *CL*s were measured using a network analyzer. The theoretical *CL* curves were simulated using Mason's equivalent circuit model.

As show in **Fig. 3(a)**, k'^2_{15} increased with increasing Sc concentration from x = 0 to 0.41. In contrast, a significant decrease of k'^2_{15} was observed for x>0.49. This decrease may be caused by the phase transition from piezoelectric wurtzite to non-piezoelectric cubic.

As shown in **Fig. 3(b)**, the V'_{44} of c-axis tilted ScAlN film decreased with the increase of Sc concentration.

The $Sc_{0.41}Al_{0.59}N$ film near the phase boundary ($0.41<x<0.49$) exhibited k'^2_{15} = 16.8% and the V'_{44} = 3851 m/s. The k'^2_{15} and V'_{44} is approximately 320 % and 60 % of that of pure AlN single with c-axis tilted angle = 30º, respectively. These piezoelectric and elastic characteristics in the ScAlN films near the phase boundary ($0.41<x<0.49$) are similar to those in a ferroelectric PZT near the phase boundary between perovskite and cubic.

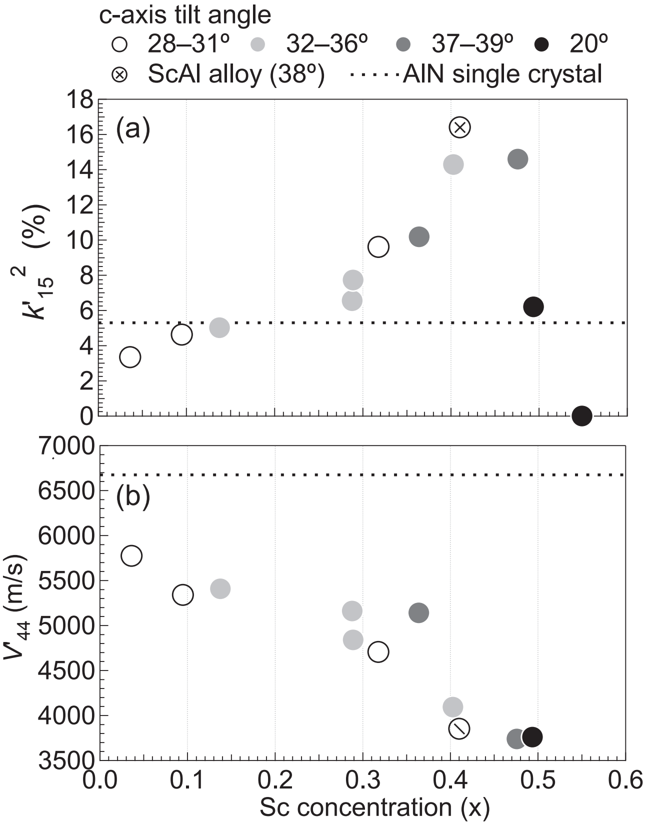

Fig. 3 The relationship between Sc concentration and (a) quasi-shear mode electromechanical coupling k'^2_{15} and (b) quasi-shear wave velocity V'_{44} in c-axis tilted $Sc_xAl_{1-x}N$ films (x=0–0.55).

4. Conclusion

c-axis tilted ScAlN films with various Sc concentration were grown by the oblique angle Sc ingot sputtering deposition. The increase of k'^2_{15} and the decrease of V'_{44} with increasing Sc concentration were observed in the c-axis tilted ScAlN films. The k'_{15} of c-axis tilted ScAlN films near the phase boundary was 3.2 times higher than that of pure AlN single crystal.

References

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