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Electromechanical coupling in ScAlN films fabricated by sputtering of Sc grain ingot
Sc 粒のスパッタにより作製した ScAlN 薄膜の電気機械結合係数

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1. Introduction

Enhancement of piezoelectric constant of d_{33} = 25 pC/N, which is more than five-fold increase compared to pure AlN, was recently found experimentally in the Sc 43% doped c-axis oriented AlN film [1]. According to this report, phase trasition from hexagonal crystal to cubic crystal occurs and piezoelectric constant reaches maximum near the 50% Sc doping. However, piezoelectric constant in this report was measured by using a DC piezometer. This piezoelectric constant seems to strongly depend on the change of the uncertain elastic or constant dielectric constant in the film. Therefore, it is important to know the electromechanical coupling coefficient (*k* value) of the film, which directly indicates conversion efficiency of electrical energy to mechanical energy.

In previous study, we have measured thickness extensional and quasi-shear mode k_{33} and k'_{15} values in the c-axis normal and tilted ScAlN films. These measurements were performed in the UHF range which is important in device application. We found that the enhancement of piezoelectricity occurs in not only the extensional mode (k_{33}) but also the quasi-shear mode (k'_{15}). Furthermore, we first reported the thickness extensional mode and shear mode ScAlN film bulk acoustic resonator (FBAR) [2].

In addition, the decrease of Q value of the FBAR due to Sc doping was recently reported by Moreira [3]. Sc and Al dual sputtering systems were used in these studies. On the other hand, we have been used single sputtering source with ScAl alloy metal target, because dual sputtering is not suitable for industrial application and considerable compositional inhomogeneity in the wafer can be exist. But, it is not easy to prepare samples with various Sc compositions in the case of ScAl alloy with constant Sc/Al ratio.

In this study, we proposed sputtering of Sc grain ingot on Al metal target by using the single sputtering source. This method allows us to investigate the effect of Sc composition on various physical constants of the film, because Sc composition can be changed by the amount of Sc ingot.

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2. ScAlN films fabrication

Two kinds of c-axis normal or tilted ScAlN film samples were prepared using a single planer RF magnetron sputtering system with 3 inch cathode. c-axis normal film sample was deposited on the well-oriented (111) Pt/Ti electrode film (400 nm)/silica glass substrate (1 mm thickness) by using ScAl alloy target sputtering. Sc composition of the alloy is 43％. c-axis tilted film sample was deposited on the Al electrode film (120 nm)/silica glass substrate (0.5 mm thickness) by using Sc grain ingot on Al metal target sputtering. Sc grain ingots with 0.2-5.0 mm, (Kojundo Chemical Laboratry, 99% purity) were put on Al target as shown in **Fig. 1**.

ScAlN film was deposited in Ar:N_2=3:1 gas, with 0.4 Pa. Substrate was cooled by a circulating water during the deposition. The distance from the target to the substrate was adjusted to 30 mm.

Film thickness of the c-axis tilted ScAlN was measured to be 4.1 μm and that of the c-axis normal ScAlN was measured to be 8.0 μm.

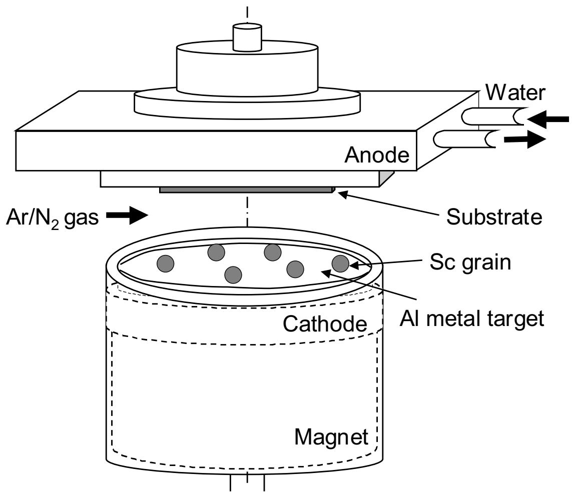

Fig. 1 Single planar RF magnetron sputtering system with Sc grain ingot on Al metal target.

3. *k* values of the ScAlN film

Au top electrode films were deposited onto both film samples, and top electrode film /piezoelectric film /bottom electrode film /substrate structure (HBAR structure) were fabricated to evaluate *k* values of the film. *k* values were determined by comparing experimental and theoretical conversion losses of the resonators [4]. Experimental conversion losses were measured by a network analyzer (Agilent Technologies E5071C) with a microwave probe. Theoretical conversion loss characteristics were calculated using modified Mason's equivalent circuit model [4]. In the c-axis tilted sample, c-axis tilt angle was predicted to be about 20-40° from the amplitude ratio of excited longitudinal wave and shear wave.

Figure. 2 shows the shear wave experimental conversion losses of c-axis tilted ScAlN film sample obtained by Sc ingot sputtering. Also shown is the theoretical conversion loss of the resonator calculated by using estimated k'_{15}. The k_{33} value of c-axis normal ScAlN film was determined by the same method.

Table. I shows the determined *k* values in c-axis normal and tilted ScAlN film, [5] single crystalline and polycrystalline pure AlN film [6] and ScAlN films. We can confirm that *k* value of c-axis normal ScAlN polycrystalline film is enhanced by Sc doping, by comparing with the *k* value of single crystalline and poly crystalline pure AlN. *k* value of the c-axis tilted ScAlN film sample deposited by present Sc ingot sputtering technique was also observed to be higher than that in single crystalline and polycrystalline pure AlN. This result shows that Sc ingot sputtering technique is effective method to study piezoelectricity enhanced ScAlN films.

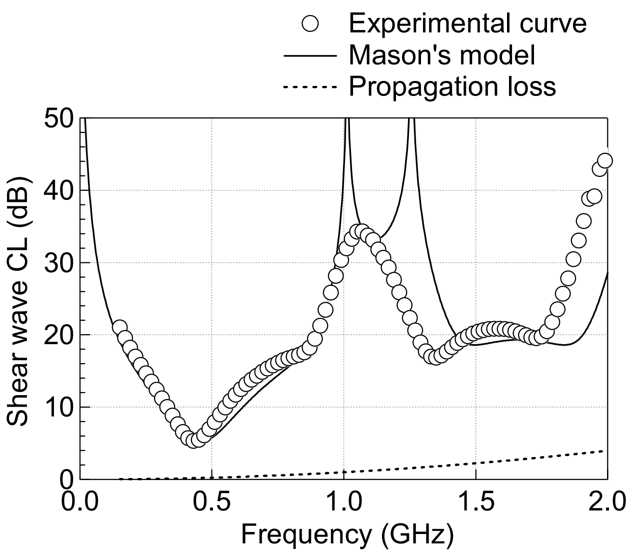

Fig. 2 Experimental and theoretical shear wave conversion loss of c-axis tilted ScAlN film resonator.

Table. I Determined *k* values in c-axis nomal and tilted ScAlN film sample. Also shown are the *k* values in single crystalline and poly crystalline pure AlN.

Orientation	c-axis normal	c-axis tilt
k value	k_{33}	k_{15}'
Sc ingot + Al plate sputtering	—	0.26
ScAl alloy plate sputtering	0.33	—
AlN (poly crystal) Ref. 5	0.17	0.14
AlN (single crystal) Ref. 6	0.30	0.23

4. Conclusions

We proposed Sc ingot sputtering technique for ScAlN film deposition. Enhancement of the *k* value was confirmed in the film deposited by our proposed technique, as well as conventional alloy sputtering technique or dual sputtering technique.

This technique will makes it possible to change Sc composition easily, even in the deposition chamber with single sputtering source. Furthermore, compositional inhomogeneity in the wafer in this technique should be smaller than dual sputtering technique.

We have not yet determined Sc composition ratio of the film fabricated by Sc ingot sputtering technique. Further research is needed to determine the Sc composition ratio of the samples.

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