1P3-5

Large electromechanical coupling (k_t^2=22%) in the ScAlN thin films

大きな電気機械結合係数(k_t^2=22%)を持つ ScAlN 薄膜

Ningrui Bai [1,2 †], Chiaki Masamune [1,2], Rei Karasawa [1,2], and Takahiko Yanagitani [1,2,3] ([1]Waswda Univ.; [2]ZAIKEN; [3]JST PRESTO)

白　寧蕊 [1,2†], 正宗　千明 [1,2], 唐澤　嶺 [1,2], 柳谷　隆彦 [1,2,3] ([1] 早稲田大学, [2] 材研, [3]JST さきがけ)

1. Introduction

Acoustic devices play an important role in cellular network technology. Comparing to other piezoelectric materials, AlN films have outstanding properties such as high acoustic velocity, and excellent Q mechanical factor [1]. These specialities make AlN can be used in acoustic resonator devices. AlN thin film bulk acoustic resonator (FBAR) filters with high frequency in mobile communication applications had already been reported [2]. Meanwhile, the low thickness extensional mode electromechanical coupling coefficient k_t^2 is a disadvantage of AlN. Doping Sc into AlN film overcomes this shortcoming. Increased piezoelectric constants of ScAlN film had been reported by Akiyama *et al.* [3]. The large bandwidth of ScAlN-based resonator [4] gets more attention in these years. The large bandwidth is own to its high k_t^2 value.

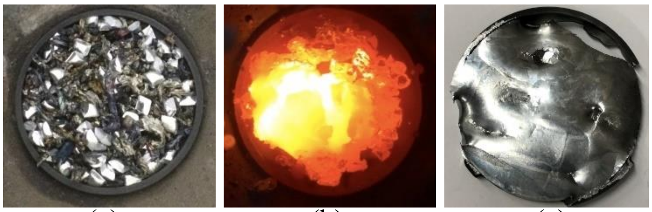
There are several sputtering methods to fabricate ScAlN films, such as dual-sputtering or single source sputtering. The dual-sputtering method uses Sc and Al targets at the same time. It is difficult to maintain concentration uniformity of Sc in large area deposition. On the other hand, ScAlN films can also be made by the single source sputtering. Two kinds of targets are usually used in single source deposition. The targets are ScAl alloy target [4] and Sc ingots on Al target [5].

Sc ingots can be easily oxidized in air. During deposition, the impact of O^- negative ions on the substrate causes worse crystallinity and piezoelectricity. This impact makes it difficult to obtain the ScAlN with high Sc concentration [6].

In this study, we compared the ScAlN films with high Sc concentration grown by using three different targets. We also measured the crystalline orientations and determined k_t^2 values of each film.

2. Targets used for depositions

Three different targets were used for fabricating ScAlN films. The first target was a 3-inch arc-melted ScAl alloy target (Sc=43atom%, Furuya metal Co., Ltd). The second target was some Sc ingots (1.1 g, Furuya metal Co., Ltd) with a 3-inch pure Al plate target. The third target was a lab-made ScAl alloy target. This target was fabricated by mixing 5.6 g of Al and 9.3 g of Sc on a carbon plate and melted by electron-beam melting (EBM) in vacuum. Sc concentration of the target was determined with an energy dispersive X-ray spectroscopy (EDX). The Sc concentration against Al was approximately 41atom%.



(a) (b) (c)

Figure 1. Typical images of (a) Al and Sc ingots placed on a carbon plate, (b) electron-beam melted ingots and (c) resulting lab-made ScAl alloy target (the third target).

3. Experiment

ScAlN films were deposited by RF sputtering on (0001) oriented Ti bottom electrode on silica glass substrates (25 × 50 × 0.5 mm) without substrate heating. Distances between substrate and targets were approximately 20 mm. The growth conditions are summarized in **Table I**.

Table I. Growth condition of the ScAlN thin films

Target	Arc-melted ScAl	Sc ingot on Al plate	EB-melted ScAl alloy
Pressure ratio	Ar: N_2=4:1		
RF power	200 W	150 W	175 W
Pre-sputtering time	1.0 hour	3.0 hours	1.0 hour
Growth time	3.5 hours	4.0 hours	6.0 hours

4. Measurement

Crystalline orientation of the films was determined by X-ray diffraction (XRD). **Table II** shows the rocking curve FWHM of each film. According to the diffraction pattern, all these ScAlN samples have (0001) preferred orientations, which means c-axis orientation is perpendicular to the

E-mail address: haku_neizui@ruri.waseda.jp, yanagitani@waseda.jp

substrate. Crystalline orientations of the films were estimated by the full width at half maximum (FWHM) of ω - scan rocking curve. As shown in Table II, all ScAlN films have good crystalline orientation. The Sc concentrations in each film are also shown in Table II. Note that there Sc concentrations measured by EDX may be under-estimated by 5 - 10%.

Table II. Data of the ScAlN thin films

Target	Arc-melted ScAl	Sc ingot on Al plate	EB-melted ScAl alloy
Rocking curve FWHM	2.1°	1.4°	2.0°
Sc concentration	32.7%	30.8%	33.2%
k_t^2 value	22.0%	14.7%	20.3%

5. Determination of k_t^2 values

Au top electrodes were deposited on the ScAlN layer to fabricate high-overtone bulk acoustic resonator (HBAR). Conversion loss (CL) was measured by a network analyser to determine the electromechanical coupling coefficient k_t^2 of each film. Measuring area on each film was the same place as EDX and XRD measurement. The theoretical CL curves were calculated by Mason's equivalent circuit model, which uses only k_t^2 value as the adjustable parameter. The k_t value can be determined by overlapping the theoretical CL curve with the experimental curve at the lowest point.

Experimental and theoretical conversion loss curves of ScAlN films are given in **Figure 2**. The sample made from arc-melted ScAl target (the first target) has the largest k_t^2 value of 22.0%. On the other hand, the sample using Sc ingots on Al target (the second target) have lower k_t^2 value than sample made from ScAl alloy. This probably dues to O^- negative ion bombardment at the substrate [6]. We prolong the pre-sputtering time for reducing the O^- ion generation at the target. The k_t^2 value of ScAlN sample using Sc ingot on Al plate target reached 14.7%. Melting ingots in high vacuum may avoid mixing oxygen into ScAl alloy. It may also prevent the O^- ion bombardment to the substrates and makes the ScAlN film have a higher k_t^2 value of 20.3%.

6. Conclusions

In this study, we found out that ScAlN film using arc-melted ScAl alloy has the world's highest k_t^2 value of 22% in the reported ScAlN films. Oxygen content in the lab-made ScAl alloy seems to be enough reduced to prevent the ion bombardment and makes k_t^2 value reached 20.3%. This value is very close to the arc-melted alloy sample. Although the film using Sc ingots has a lower k_t^2 value than other samples, it is still a large electromechanical coupling coefficient value about 14.7%. All these ScAlN films have higher k_t^2 values than past report by our group [5].

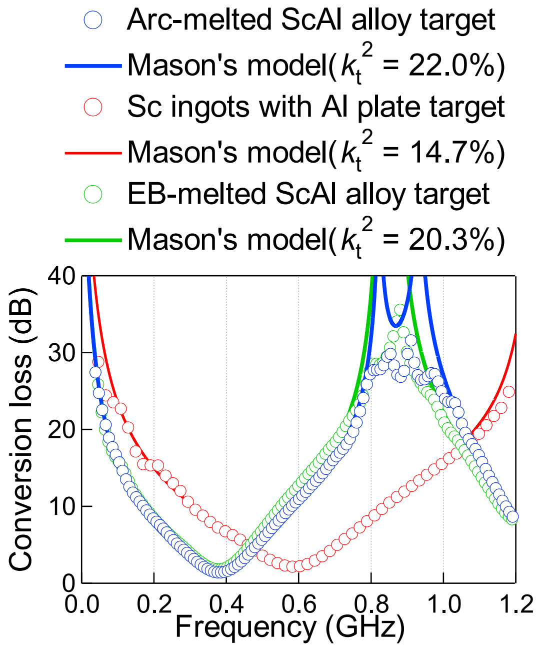


Figure 2. Experimental and theoretical conversion loss curves of ScAlN films made by Arc-melted ScAl alloy target, Sc ingots with pure Al plate target, and electron-beam melted ScAl alloy target. The theoretical curves were simulated by Mason's equivalent circuit model including the electrode layers.

Acknowledgement

This work was supported by JST PRESTO (No. JPMPPR16R8), JSPS KAKENHI (Grant-in-Aid for Scientific Research (B), No. 16H04356), and ZAIKEN.

References

1. K. M. Lakin, in Proc. IEEE Ultrason. Symp., pp. 895-906, (1999)
2. T. Nishihara, T. Yokoyama, T. Miyashita, Y. Satoh, in Proc. IEEE Ultrason. Symp., pp. 969-972, (2002).
3. M. Akiyama, T. Kamohara, K. Kano, A. Teshigahara, Y. Takeushi, N. Kawahara, Adv. Mater. 21, 593, (2008).
4. T. Yanagitani, K. Arakawa, K. Kano, A. Teshigahara, M. Akiyama, in Proc. IEEE Ultrason. Symp., pp. 2095-2098, (2010).
5. T. Yanagitani, M. Suzuki, Appl. Phys. Lett., 105, 122907, (2014).
6. S. Takayanagi, M. Matsukawa, T. Yanagitani, in Proc. IEEE Ultrason. Symp., 7728836, (2016).