Effect of negative ions generation from sputtering target on crystalline orientation and k_t^2 of ScAlN thin films

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Abstract—Large electromechanical coupling coefficient k_t^2 of the piezoelectric thin film is required for wide band operation in the bulk acoustic wave (BAW) filter. k_t^2 of AlN thin film was greatly improved by Sc doping. Sc metal usually contains carbon and oxygen impurities. Therefore, CN⁻ and O⁻ negative ions are generated from Sc sputtering target. As a result, crystalline orientation is degraded due to these negative ions bombardment to the substrate. We know that negative ions generation increase with increasing target temperature. In this study, to suppress negative ions generation from the target, Sc grains were embedded in water cooled Al metal disc target. ScAlN thin films were grown by RF magnetron sputtering. Two types of targets, where Sc grains are just put (heated) or those are embedded (cooled), are compared.

Keywords—ScAlN, piezoelectric thin film, negative ion, electromechanical coupling coefficient

I. INTRODUCTION

With the development of wireless devices in recent years, BAW (bulk acoustic wave) filters which have wide band and sharp frequency characteristics are demanded for high speed and massive capacity wireless network. Large electromechanical coupling coefficient k_t^2 of the piezoelectric thin film is required for wide band operation in the BAW filter. AlN thin films are used in smartphones as FBAR (film bulk acoustic resonator) filters. However, piezoelectric film whose k_t^2 is larger than AlN film (k_t^2 = 6.5% [1]) is demanded. Therefore, ScAlN thin films began to be used in new type of smartphones because k_t^2 of AlN thin films were greatly improved by Sc doping (k_t^2 =18.5%) [2,3]. The piezoelectricity of ScAlN film improves as Sc concentration increases until it reaches 43% [2].

In previous studies, we reported that crystalline orientations of ScAlN thin films were degraded due to CN⁻ and O⁻ negative ions bombardment to the substrate during the sputtering growth [4,5]. Sc metal usually contains carbon impurity because of Sc melting process with carbon crucible. Sc metal also contains oxygen due to their high oxygen affinity. Therefore, CN⁻ and O⁻ negative ions are generated from Sc sputtering target. In this study, to suppress negative ions generation from the sputtering target, Sc grains were embedded in 2 inches Al metal disc target. Al metal disc target was cooled by water circulating cathode during the sputtering growth. Therefore, Sc grains embedded in Al metal disc are cooler than just put Sc grains on Al metal disc because of the difference in cooling effect by water.

II. FABRICATION OF SCALN THIN FILMS

We used two types of sputtering targets, where Sc grains are just put (heated) or those are embedded (cooled), as shown in Fig. 1. To investigate the effect of cooling Sc ingots, two types of ScAlN thin films were grown on (0001) oriented Ti bottom electrode/ silica glass substrate by RF magnetron sputtering. highly oriented Ti films (rocking curve full-width at halfmaximum (FWHM) are approximately 2.0°) were fabricated by DC magnetron sputtering. These ScAlN films were grown under the same sputtering condition. Fig. 2 shows the RF magnetron sputtering system and Table I shows sputtering condition. To adjust Sc concentration of two ScAlN thin films, we used 35 Sc grains for heated target and 70 Sc grains for cooled target. The size of Sc grains was approximately $5 \times 5 \times 5$ mm³.

The oxygen and carbon impurities in Sc ingots were measured by infrared absorption spectroscopy (EMGA-930, Horiba and CS844, LECO). Sc grains for cooled target and heated target contained approximately 2600 ppm and 1700 ppm oxygen impurities, respectively. These Sc grains contained too low carbon impurities to detect (approximately 0 ppm).

The temperature of Sc grains on erosion position was measured by a radiation thermometer during sputtering. The average temperature of heated and cooled Sc grain target was approximately 670 °C and 580 °C, respectively.

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Fig. 1 Two types of sputtering targets : heated Sc grains and cooled Sc grains.



Fig. 2 RF magnetron sputtering system.

Table I Sputtering condition of ScAlN thin films

| Total pressure | < 10 ⁻⁴ Pa |
|----------------------------|-----------------------|
| Gas pressure | 0.5 Pa |
| Ar/N ₂ | 4 |
| RF power | 150 W |
| Deposition time | 4.5 hours |
| Presputtering time | 1 hours |
| Substarate-target distance | 22 mm |
| Substrate heating | None |

III. MESUREMENT OF NEGATIVE IONS ENERGY

Energy of negative ions bombardment was measured by an energy analyzer with Q-mass (PSM003, Hidden Analytical) during sputtering. The energy analyzer was installed at the same position as the substrate position. In previous study, the intensity of CN^- was larger than that of O^- [4]. Therefore, we measured energy distribution of CN^- negative ions. As a result, the suppression of the CN^- ion irradiation by cooling of the Sc grains was observed, as shown in Fig. 3. In addition, we found that energy of CN^- bombardment was decreased by extending presputtering time.



Fig. 3 CN⁻ negative ions flux and energy distribution generated by two types of targets.

IV. EVALUATION OF SCALN THIN FILMS

A. Crystalline orientations

The crystalline orientation of ScAlN thin films were evaluated by the X-ray diffraction (XRD (PANalytical, X'Pert Pro MRD)). Fig. 4 shows 2θ - ω scan XRD patterns. (0002) orientation were observed in the ScAlN thin films grown by heated and cooled Sc grains. Fig. 5 shows the ω -scan rocking curve of the two ScAlN films measured by XRD. The rocking curve FWHM (0002) of the ScAlN thin films grown by heated and cooled Sc grains was 2.1° and 1.4°, respectively. The rocking curve FWHM and integrated intensity of the ScAlN thin film with cooled Sc grains was better than that of the film with heated Sc grains.



Fig. 4 2θ - ω scan XRD patterns of ScAlN thin films grown by heated and cooled Sc grains.



Fig. 5 The rocking curves of ScAlN thin films grown by heated and cooled Sc grains.

B. Electromechanical coupling coefficient k_t^2

The k_t^2 of ScAlN thin films were evaluated by comparing experimental conversion loss (*CL*) and theoretical *CL* of ScAlN thin films. Experimental *CL* were measured by a network analyzer (E5071C, Agilent Technologies), as shown in Fig. 6. Fig. 7 shows experimental *CL* curves. Theoretical *CL* which were calculated by a Mason's equivalent circuit model is also shown in Fig. 7. k_t^2 of the ScAlN thin films grown by heated and cooled Sc grains were 18.0% and 19.3%, respectively. k_t^2 of the ScAlN thin film with cooled Sc ingots was better than that of the film with heated Sc ingots.

Table II shows the characteristics of ScAlN thin films fabricated by two types of targets. The thickness and Sc concentration of ScAlN thin films was measured by a stylus profiler and X-ray fluorescence analyzer (XRF), respectively.



Fig. 6 Measurement system of experimental *CL* by the network analyzer.



Fig. 7 Conversion loss curves of ScAlN thin films grown by heated and cooled Sc grains.

Table IICharacteristics of ScAlN thin films fabricated bytwo types of sputtering target: heated Sc grains and cooled Scgrains.

| | Thickness of film (µm) | Sc concentration (atom %) | Rocking curve FWHM | $k_{\rm t}^2$ |
|----------------------------------------|------------------------------|---------------------------------|--------------------------|---------------|
| ScAlN film (heated Sc grains) | 5.1 | 33% | 2.1° | 18.0% |
| ScAlN film (cooled Sc grains) | 6.1 | 31% | 1.4° | 19.3% |

V. CONCLUSION

Electromechanical coupling coefficient k_t^2 and crystalline orientation of ScAlN thin films were improved by using embedded (cooled) Sc grains target because of the suppression of negative ions generation by cooling. Larger k_t^2 of ScAlN thin film can be obtained by increasing Sc concentration. The difference between the two types of targets can be more clear by comparing more thin ScAlN films. In the future, a new growth method to suppress negative ions bombardment to the substrate is required.

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