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Increase of electromechanical coupling coefficient in c-axis oriented AlN films by chromium doping at low concentrations

低濃度 Cr ドープによる c 軸配向 AlN 薄膜の電気機械結合係数増幅

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1. Introduction

AlN films have high velocity and low acoustic attenuation. Therefore, AlN film bulk acoustic wave resonators (FBARs) are used as frequency filters in mobile communications. However, AlN FBARs possess rather small electromechanical coupling coefficient k_t^2, which lead narrow band width in filter applications.

In 2018, S. Manna *et al*. theoretically demonstrated that doping Cr in AlN films increases piezoelectric constant d_{33} [1]. In USE2019, we experimentally demonstrated that the k_t^2 in GHz range was improved in CrAlN films [2]. We grew $Cr_{0<x<0.21}Al_{1-x}N$ films by RF magnetron sputtering deposition. A highly oriented film was successfully grown at Cr concentration of 4% or less. The k_t^2 was 5.6% at Cr concentration of 1%, which was approximately 1.2 times of that of a pure AlN film. However, we reproducibly could not grow the CrAlN films with high k_t^2. In addition, film growth conditions were not optimized for CrAlN films.

In this study, we mainly fabricated CrAlN films with low Cr concentration, which is expected to increase k_t^2. In addition, we investigated suitable film growth conditions for CrAlN films such as water temperature for cooling target and insertion of AlN intermediate layers.

2. CrAlN films growth

CrAlN films were grown by RF magnetron sputtering system as shown in **Fig. 1**. We placed Cr metal ingots (99.9 %, Kojundo chemical Lab. Co. Ltd.) on the Al metal target (99.9%, Furuuchi chemical) to dope Cr in AlN films. The amount of Cr ingots on the Al target was adjusted to be 0-1.0 g for the control of Cr concentrations in the films. (0001) oriented Ti bottom electrode films (400-700 nm) were grown on silica glass substrates (0.5 mm).

It was reported that negative ion irradiation to the films during sputtering films growth causes deterioration of crystallinity [3]. In ScAlN film growth, negative ion irradiations can be suppressed

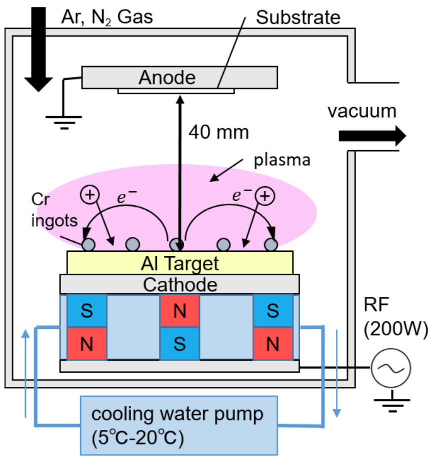

Fig.1 The schematic of RF magnetron sputtering apparatus.

by cooling Sc ingots on the Al metal target [4]. Therefore, in CrAlN film growth, water temperature for cooling Al target and Cr ingots was changed from 20°C (in USE2019) to 5°C.

In addition, we also investigated the effect of insertion of AlN intermediate layers between CrAlN film and Ti film on the properties of CrAlN films. We grew highly oriented pure AlN intermediate layers (300 nm) on Ti films. Base pressure, gas pressure, N_2 : Ar gas ratio, RF power, distance form target to substrate, and substrate temperature were set to be $<10^{-3}$ Pa, 0.75 Pa, 1 : 2, 200 W, 40 mm, room temperature, respectively. The Cr concentrations in the CrAlN films were determined by an Electron Probe Micro Analyzer (JEOL, JXA-8200).

3. Crystalline orientation

We evaluated crystal orientation by a XRD analysis (Rigaku, JDX-3530). **Fig. 2** shows 2θ-θ XRD patterns of samples with pure AlN film, CrAlN film reported in USE2019, the film with cooling target of 5°C and the film with insertion of AlN intermediate layer. The Cr concentrations of the samples were 1-2%. (0002) AlN peaks were

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observed about 36º in all samples. Rocking Curve FWHM (R.C. FHWM) of (0002) AlN peak is 2-4 º in all samples. (111) CrN or (002) Cr_2N peak around 40º, which appeared in the samples of previous report, was not observed in this study's samples. However, at present, we have seen no reason why (111) CrN or (002) Cr_2N peak was disappeared.

4. Piezoelectric characteristics

In order to estimate the piezoelectric characteristic of CrAlN films, HBAR structures were prepared by evaporating Au or Cu top electrode films on CrAlN films surface. The k_t^2 and longitudinal wave velocity V_L were determined by comparing the conversion loss curve of HBAR measured by a network analyzer (Agilent Technologies, E5071B) and the theoretical curve calculated by Mason's equivalent circuit model. As shown in **Fig. 3**, the k_t^2 of CrAlN films at low Cr concentrations of less than 2% are higher than that of pure AlN film. In addition, we observed increase of k_t^2 in several CrAlN films samples. In particular, the k_t^2 of 5.9% with a Cr concentration of 1.2% was approximately 1.3 times higher than that of the pure AlN film. The k_t^2 decreased with increasing Cr concentrations of more than 4%. The V_L decreased with increasing Cr concentration.

The k_t^2 of CrAlN films with cooling target of 5 ºC was better than that in sample with cooling target of 20 ºC (USE2019). We consider that this improvement of k_t^2 are due to the suppression of no piezoelectric (111) CrN or (002) Cr_2N grain growth. In contract, the insertion of AlN intermediate layer did not affect the k_t^2. Therefore, the cooling target strongly lead to improve crystal orientation and piezoelectric characteristic of CrAlN films.

Table 1 shows k_t^2 values of pure AlN, CrAlN, and ScAlN films determined from characteristic of HBAR. At high doping concentrations, CrAlN film did not excite bulk waves, but ScAlN film had high k_t^2 of 7.4%. On the other hand, at low doping concentrations, the k_t^2 of 5.9% at Cr concentration of 1.2% in this report was higher than that of 4.8% at Sc concentration of 5%. Therefore, Cr doping may be substituted for Sc doping at low doping concentrations.

5. Conclusion

C-axis oriented CrAlN films with low Cr concentrations were grown in several conditions. Crystal orientation and k_t^2 of CrAlN films were improved by cooling target. The k_t^2 of 5.9% was approximately 137% of that of pure AlN film.

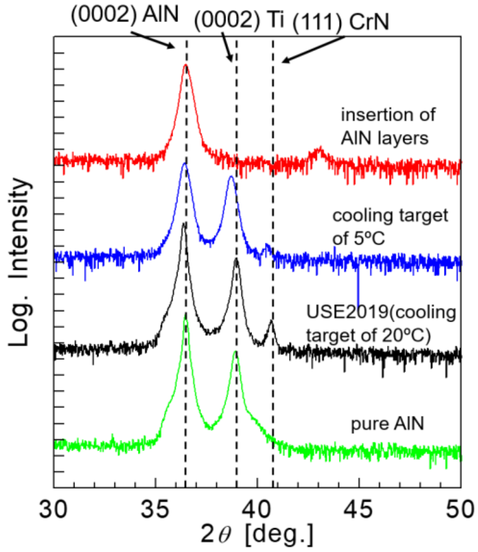

Fig. 2 XRD patterns of AlN or CrAlN films.

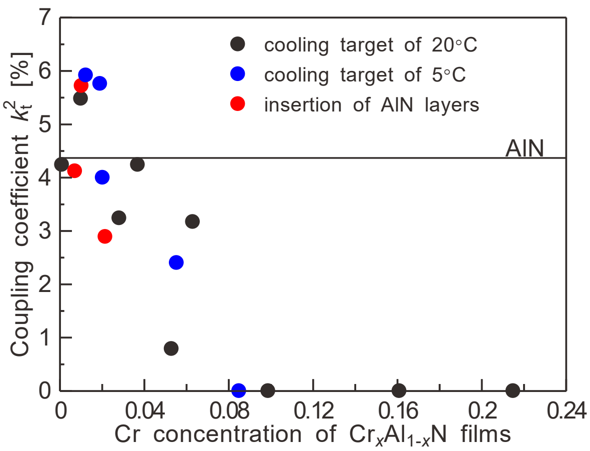

Fig. 3 k_t^2 as a function of Cr concentrations x.

Table I k_t^2 of pure AlN, CrAlN and ScAlN films.

	AlN	CrAlN		ScAlN [5]	
conc.	---	1.2%	21%	5%	28%
k_t^2	4.3%	5.9%	---	4.8%	7.4%

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