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Electromechanical Coupling Coefficient k_t^2 of Cr doped AlN Films Grown by Sputtering Deposition

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***Abstract*— Electromechanical coupling coefficients of ScAlN films are higher than those of other wurtzite piezoelectric films. Therefore, ScAlN films have attracted attention as a new piezoelectric layer in BAW resonators. However, Sc target for ScAlN film sputtering growth are very expensive because scandium is rare earth material. Recently, enhancement of d33 in Cr doped AlN film was found theoretically and experimentally. In this study, we investigated kt2 and longitudinal wave velocity for GHz range in c-axis oriented Cr0<x<0.16Al1-xN films. c-Axis oriented CrAlN films were grown by Cr ingot RF sputtering deposition. Cr concentration in CrAlN film were controlled by varying the amount of Cr ingots on Al target. kt2 and longitudinal wave velocity were estimated from a longitudinal wave conversion loss in CrAlN film HBARs with Cu/CrAlN/Ti/Silica glass substrate. The kt2 of 5.5 % in Cr0.01Al0.99N film was approximately 1.2 times higher than that in pure AlN film. On the other hand, the kt2 significantly decreased with increasing Cr concentration from 0.04 to 0.16. This decrease of kt2 may be due to the low crystalline orientation or the phase transition from a piezoelectric to a non-piezoelectric crystal phase. In addition, the longitudinal wave velocity decreased with increasing Cr concentration.**

Keywords—AlN film bulk acoustic wave resonator, Cr doped AlN film, electromechanical coupling coefficient

I. INTRODUCTION

AlN film bulk acoustic wave resonators (FBARs) have high Q factor and can operate at high frequency. Therefore, AlN FBARs are used as frequency filters in mobile communications. However, the relatively small electromechanical coupling coefficient k_t^2 in AlN FBAR causes a narrow band width in filter applications.

M. Akiyama *et al.* demonstrate that piezoelectricity of wurtzite AlN films are increased by doping scandium (Sc) with the AlN films [1]. The d_{33} of the $Sc_{0.43}Al_{0.57}N$ films is approximately five times higher than that of pure AlN film. In addition, this enhancement of piezoelectricity in Sc doped AlN films was demonstrated theoretically by a density functional theory [2,3]. Then, the characteristics of Sc doped AlN FBAR have been reported [4-8], because there is a possibility that the high piezoelectricity in Sc doped AlN films leads to the increase of k_t^2 in AlN FBARs. The k_t^2 in Sc doped AlN films increased with increasing Sc concentration. The k_t^2 of 18.5 % in $Sc_{0.4}Al_{0.6}N$ films is approximately 200 % of that in a pure AlN single crystal. On the other hand, the decrease of longitudinal wave velocity and Q factor were observed in Sc doped AlN films. The degradation of crystalline orientation due to ion bombardments from Sc target during film growth was also observed. Moreover, the cost of Sc doping is very expensive because Sc is rare earth materials.

After that, the increases of piezoelectricity and electromechanical coupling coefficient by doping metal element with wurtzite AlN film were demonstrated continuously. In 2014, T. Yokoyama *et al.* (Taiyo Yuden Co.,Ltd) found the increase of electromechanical coupling coefficient in MgZrAlN FBAR [10]. Mg and Zr is cheaper than Sc, but Mg and Zr concentration control is more difficult than Sc doping. In 2018, S. Manna *et al.* demonstrated the enhancement of piezoelectric constant d_{33} in Cr doped AlN films [11]. The cost of Cr doping is much cheaper than that of Sc doping. Moreover, Cr doped AlN films may be obtained by same deposition techniques as ScAlN film deposition. However, piezoelectric properties in GHz range of CrAlN FBARs have not been reported.

In this study, we fabricated c-axis oriented Cr doped AlN films by using Cr ingot RF sputtering deposition. The crystalline orientation of the CrAlN films were estimated by XRD analysis. The effects of Cr doping with AlN films on k_t^2 and longitudinal wave velocity were investigated from the frequency characteristics of longitudinal wave conversion losses in CrAlN film HBARs.

II. CRALN FILM GROWTH

c-Axis oriented CrAlN films were grown by using Cr ingot RF magnetron sputtering deposition shown in Fig. 1. Cr ingots (99.9 %, Kojundo chemical Lab. Co. Ltd.) were placed on Al target (99.99 %, Furuuchi Chemical). The Cr ingots and Al target were sputtered simultaneously, and CrAlN films grow on the substrate. In order to obtain CrAlN films with various Cr concentration, the total amount of Cr ingots were adjusted to be 0, 0.1, 0.25, 0.5, 1.0 g. As shown in Table I, (0001) oriented Ti bottom electrode films (200-700 nm) on silica glass substrates were used as the substrates to obtain highly c-axis oriented CrAlN film. The film thickness of the CrAlN films were 3-5 μm. The Cr concentration in the $Cr_xAl_{1-x}N$

films was determined to be x=0-0.16 by an electron probe micro analyzer (JXA-8200, JEOL).

III. CRYSTALLINE ORIENTATION OF CRALN FILMS

We estimated the crystalline orientation of AlN and CrAlN films by using an XRD analysis. Fig. 2 shows 2θ-θ XRD patterns of the samples. (0002) AlN peaks around 36º, indicating that c-axis is normal to the substrate surface, were observed in all samples. The XRD intensity of (0002) AlN peaks decreased with increasing Cr concentration. Fig. 3 shows the c-axis lattice length $d_{(0001)}$ of CrAlN films as a function as Cr concentration. The $d_{(0001)}$ was determined from

$$d_{(0001)} = \frac{\lambda}{\sin(\theta_{(0002)})} \quad (1)$$

where λ and $\theta_{(0002)}$ indicate the CuK_α X-ray wave length (1.5418 Å) and the angle of (0002) AlN peak, respectively. The $d_{(0001)}$ increased with increasing Cr concentration. The increase of $d_{(0001)}$ was also observed in ScAlN films, and may causes the enhancement of piezoelectricity. Fig. 4 shows the rocking curve full width half maximum (R.C. FWHM) of (0002) AlN peaks in the samples. The values of R.C. FWHM in Cr concentration x=0.00-0.04 were estimated to be 2.2-2.8. The crystalline orientation is good in $Cr_xAl_{1-x}N$ film with Cr concentration x<0.04. On the other hand, the values of R.C. FWHM in Cr concentration x>0.06 were more than 5º.

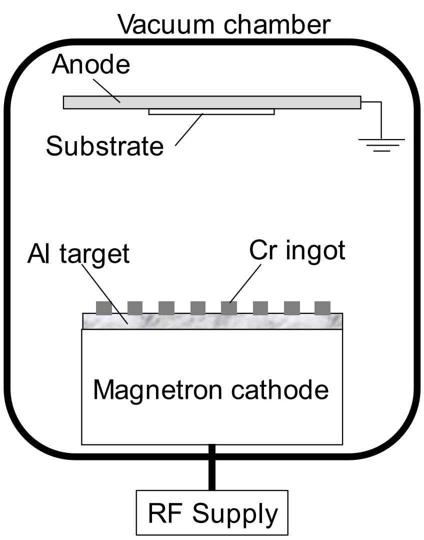

Fig. 1 Cr ingot RF magnetron sputtering deposition.

Table I Film growth conditions.

Base pressure	$<10^{-3}$ Pa
Gas Pressure	0.75 Pa
Ar:N_2 gas ratio	2:1
RF power	150-200 W
Al Target size	3 inch
Cr ingots	0-1.0 g
Substrate	(0001) Ti/Silica glass substrate
Distance from target to substrate	40 mm
Film thickness	3-5 μm

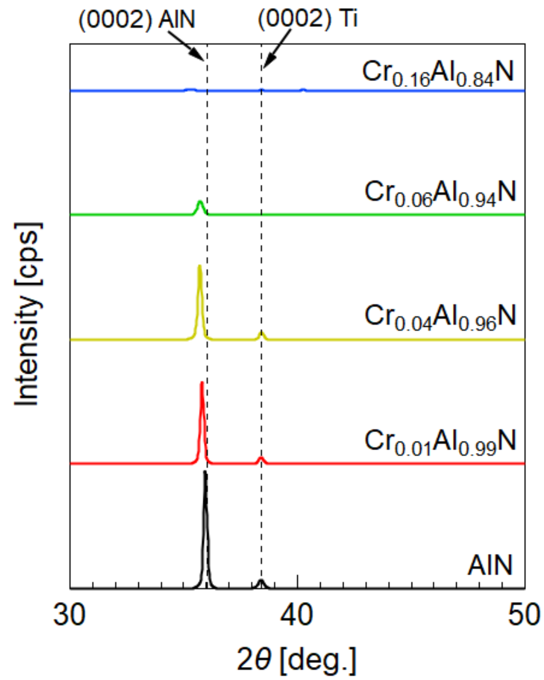

Fig. 2 2θ-θ XRD patterns of CrAlN film samples.

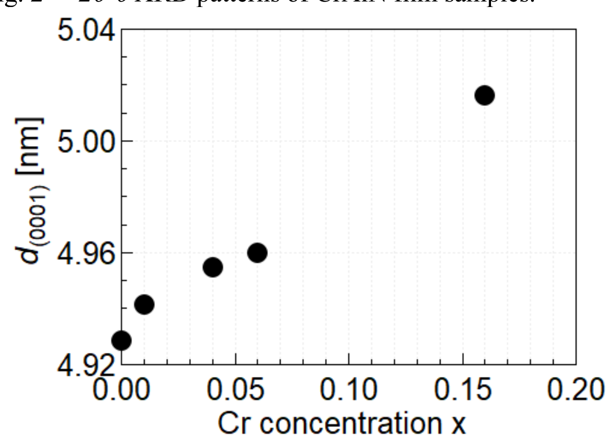

Fig. 3 c-axis lattice length of $Cr_xAl_{1-x}N$ films as a function of Cr concentration x.

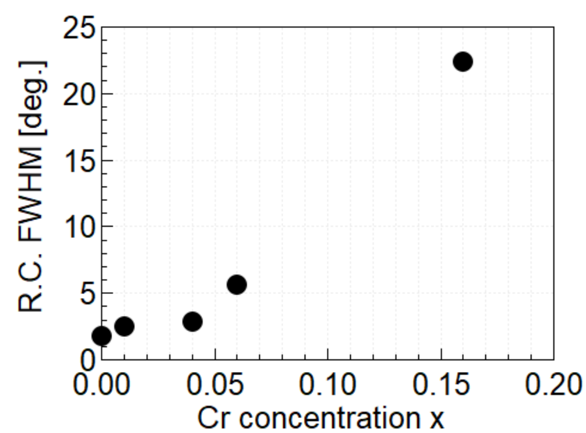

Fig. 4 Rocking curve FWHM (R.C. FWHM) of (0002) CrAlN peak in $Cr_xAl_{1-x}N$ films as a function of Cr concentration.

IV. Piezoelectric properties of CrAlN films

In order to obtain high overtone bulk acoustic wave resonators (HBARs), we fabricated Cu top electrode films (100-400 nm) on CrAlN film/Ti bottom electrode film/silica glass substrate by using a vacuum evaporation method. The frequency characteristics of the longitudinal wave conversion losses in the HBARs were measured by a network analyzer (Agilent Technologies, E5071B). The electromechanical coupling coefficient k_t^2 and longitudinal wave velocity V_L were determined from comparing the experimental conversion loss curve with theoretical curve, calculated by a Mason's equivalent circuit model. The density and dielectric constant of an AlN single crystal [12] were used as that of CrAlN films in the Mason's model. Fig. 5 shows the longitudinal wave conversion loss of the HBAR consisting of Cu top electrode film/$Cr_{0.01}Al_{0.99}N$ film/Ti bottom electrode film/silica glass substrate. The k_t^2 and V_L of $Cr_{0.01}Al_{0.99}N$ film were estimated to be 5.5% and 9,400 m/s, respectively. Fig. 6 shows the k_t^2 of CrAlN films as a function of Cr concentration. The k_t of $Cr_{0.01}Al_{0.99}N$ film is approximately 1.2 times higher than that of 4.4% in pure AlN films with high orientation. On the other hand, the k_t of $Cr_{x>0.04}Al_{1-x}N$ films were smaller than that of pure AlN films and decreased with increasing Cr concentration. In addition, we did not observed the longitudinal wave excitation in $Cr_{0.16}Al_{0.84}N$ film HBARs. As shown in Fig. 2, the XRD intensity of (0002) AlN peak in the $Cr_{0.16}Al_{0.84}N$ film is much smaller than those in AlN films and CrAlN films with low Cr concentration. From these results, we consider that the crystal phase of $Cr_{0.16}Al_{0.84}N$ film may be changed from a piezoelectric wurtzite phase to a non-piezoelectric phase. Fig. 7 shows the relationship between V_L and Cr concentration in CrAlN films. The V_L decreased with increasing Cr concentration. This decrease of V_L by doping metal elements was also observed in ScAlN films and MgZrAlN films with high electromechanical coupling coefficients.

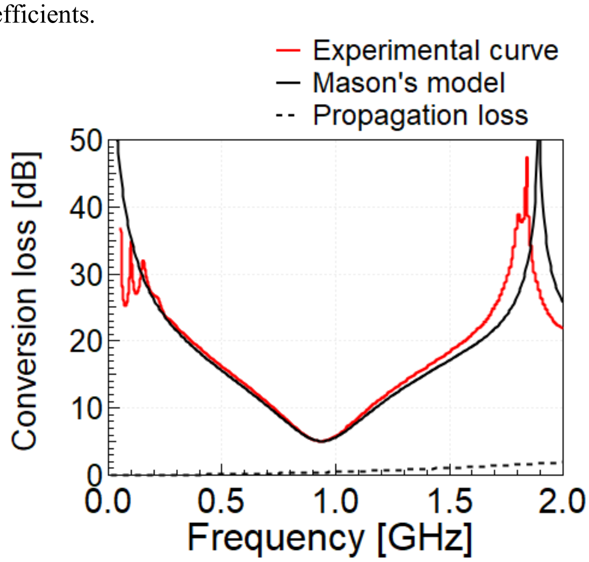

Fig. 5 Longitudinal wave conversion loss of HBAR consisting of Cu/$Cr_{0.01}Al_{0.99}N$/TI/silica glass substrate.

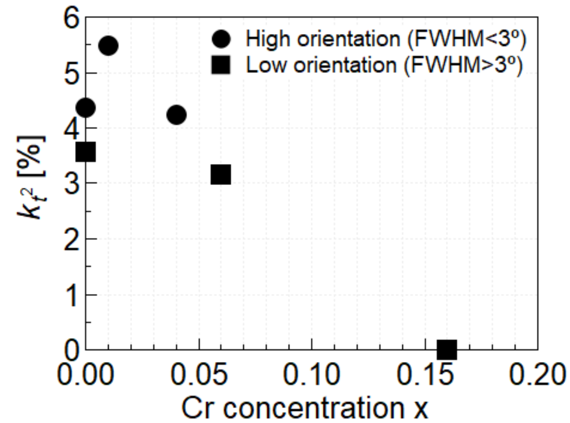

Fig. 6 Electromechanical coupling coefficient k_t^2 of $Cr_xAl_{1-x}N$ films as a function of Cr concentration x.

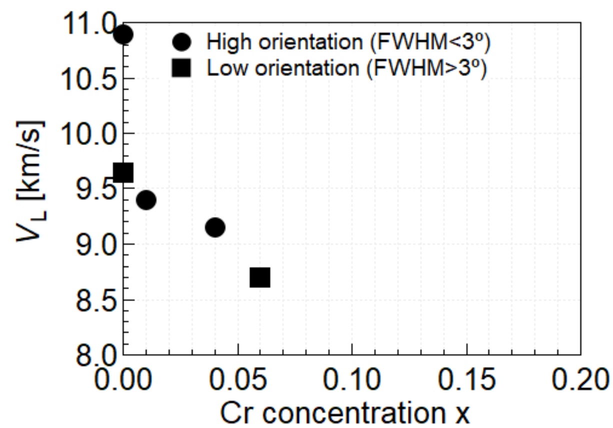

Fig. 7 Longitudinal wave velocity V_L of $Cr_xAl_{1-x}N$ films as a function of Cr concentration x.

V. Conclusion

c-Axis oriented $Cr_{0<x<0.16}Al_xN$ films with various Cr concentration were grown by Cr ingot RF sputtering deposition. The relationship between electromechanical coupling coefficient k_t^2 or longitudinal wave velocity V_L and Cr concentration in CrAlN films was investigated from the longitudinal wave conversion losses of CrAlN HBARs. The k_t^2 enhanced in CrAlN films with low Cr concentration. The k_t^2 of 5.5% in $Cr_{0.01}Al_{0.99}N$ film was approximately 120% of that in pure AlN film. The V_L decreased with increasing Cr concentration.

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