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Giant shear mode electromechanical coupling in c-axis tilted ScAlN films

c 軸傾斜配向 ScAlN 膜の擬似すべりモードおける巨大圧電性

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1. Introduction

Significant increase of piezoelectricity was recently found experimentally in the Sc heavily doped AlN film [1]. Theoretical prediction based on density-functional theory was also consistent with the experimental results [2]. Fifth fold increase of extensional piezoelectric constant d_{33} value, compared to the AlN film, was observed in the $Sc_{0.43}Al_{0.57}N$ alloy films [1]. However, piezoelectric characterization in these studies were based on direct current measurement using a piezo-meter. To use these films in BAW and SAW applications, it is important to know the electromechanical coupling, k values in the microwave frequencies. In addition, it is interesting to investigate the shear mode properties in the ScAlN films.

In this study, we present the quasi-thickness extensional mode and quasi-thickness shear mode electromechanical coupling coefficient k_{33}' and k_{15}' values in the c-axis tilted ScAlN films.

On the other hand, piezoelectricity in most of the ferroelectric material, for example, PZT and $BaTiO_3$ deteriorates above 500 ºC due to phase transition. Piezoelectricity starts to deteriorate at 600 ºC even in $LiNbO_3$ which possesses high T_c [3]. ScAlN film have a potential to sustain large piezoelectricity at high temperature. Here, electromechanical properties of the films in 600 ºC are also presented and compared with c-axis tilted ZnO films which possess highest k values in the wurtzite.

2. Method

2.1 c-axis tilted ScAlN films

c-axis tilted ScAlN films (1.5–3 μm) were deposited on Al/silica glass substrate using a planar RF magnetron sputtering system. ScAl alloy metal with 37% Sc concentration was used as a target. Two samples A and B with different c-axis tilt angle and degree of orientation were prepared. An electron probe micro analysis (EPMA) showed that Sc/Al composition ratio in the alloy films were in accordance with that in the target alloy.

2.2 Crystalline orientation and piezoelectric properties in the film

First, crystalline orientation of the films was investigated by using a 0002 plane pole figure analysis. c-axis tilt angle and the degree of the crystalline orientation were determined from the peak value and FWHM value of the a ψ-scan profile curve of the 0002 pole.

Next, copper top electrode films were deposited onto film samples, and composite resonator structure were fabricated. k_{33} and k_{15} values of the film layer were determined by comparing experimental and theoretical conversion losses of the resonators [4, 5]. Theoretical conversion loss characteristics were calculated using modified Mason's equivalent circuit model including effect of c-axis tilt and electrode layers [6].

In addition, k values were measured at 25-600 ºC in air by using heating/cooling stage (Linkam, LK-600PH). Top copper electrode film was removed and high temperature tolerant Pt or Au top electrode film was Dc-sputter-deposited.

3. Results

3.1 Crystalline orientation

Figure 1 shows the typical 0002 pole figure of the ScAlN film (sample A). c-axis tilt angle is found to be 19º. ψ–scan FWHM of pole is measured to be 8.5º, indicating relatively high crystalline orientation. In sample B c-axis tilt angle and ψ–scan FWHM are measured to be 14º and 6.7º, respectively.

3.2 Piezoelectric properties

Figure 2 shows the calculated k_{33}' and k_{15}' values as a function of c-axis tilt angle γ in pure single crystalline AlN. Physical constant of AlN reported by Ohasi [7] was used in the calculation. We have plotted determined k_{33}' and k_{15}' values in the Fig. 2. Both values in polycrystalline ScAlN films far

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exceeded that in single crystalline AlN. Large k_{15}' value of 0.35 k_{15}^2=12 %) was obtained in sample A. k_{15}' values of the AlN increased with increasing c-axis tilt angle. This tendency implies that further high k_{15} value is expected if 30º tilted film is obtained.

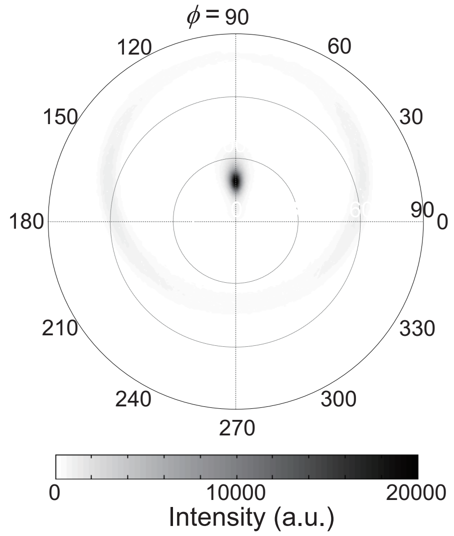

Fig. 1 (0002) pole figure in the ScAlN film (sample A)

3.3 k values in high temperature

Figures 3 shows the temperature characteristics of k_{33}' and k_{15}' values in the c-axis tilted ScAlN samples. Characteristics for c-axis non-doped AlN films [8] and c-axis tilted ZnO film [6] are also displayed in the figures. In the ZnO film, both k_{33}' and k_{15}' values started to decrease at 400 ºC, probably due to the increase of n-type conductivity [9] caused by increase of oxygen vacancy. k values recovered to the value at room temperature when sample was cooled. In contrast, significant deterioration of k value was not observed in the c-axis tilted AlN and ScAlN films. Large hysteresis characteristic did not appear in all samples. We could not perform the measurement above 600 ºC because of the specification limit of the heating stage. Perhaps, ScAlN films can be used in higher temperature.

4. Conclusions

Giant electromechanical coupling k_{33}' and k_{15}' of 0.35 (k_{15}^2=12 %) were found in the c-axis 19º tilted ScAlN films. Higher k_{15} value is expected if 30º tilted film is obtained. High k values were observed even in the high temperature of 600 ºC.

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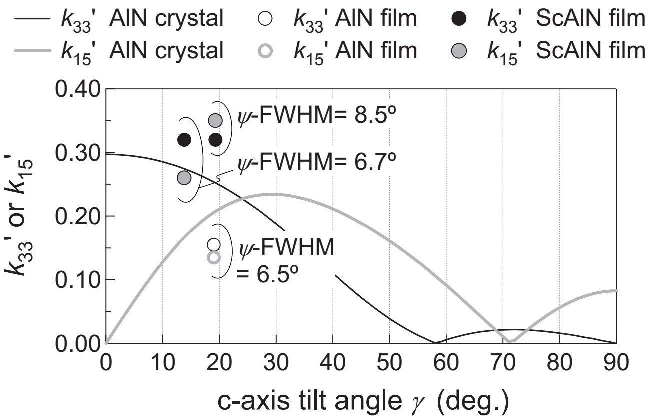

Fig. 2 Calculated k'_{33} and k'_{15} values of single-crystalline AlN as a function of the c-axis tilt angle. Also plotted are experimentally determined k values of the ScAlN films at each c-axis tilt angle determined by pole figure analysis.

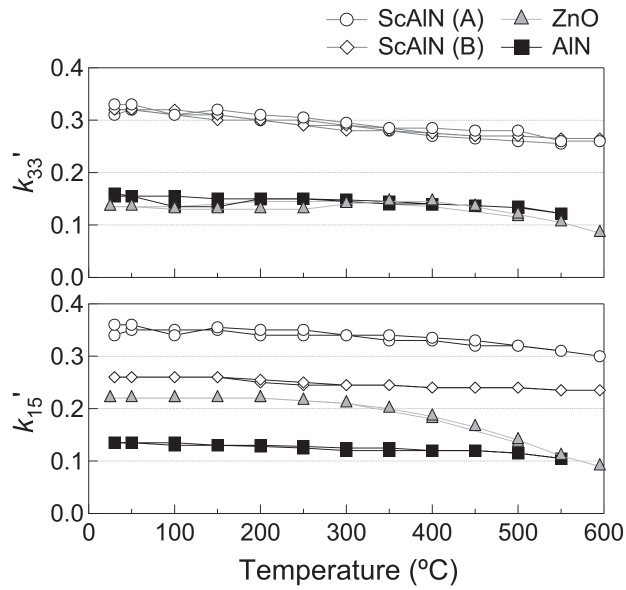

Fig. 3 k values as a function of the temperature for the c-axis tilted ScAlN films and c-axis tilted ZnO films and AlN films for a comparison.