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Temperature coefficient of elastic and GHz piezoelectric properties in ScAlN films
ScAlN 膜における相境界付近の GHz 帯圧電特性と弾性温度係数

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1. Introduction

AlN has high velocity, Q factor, power handling capability, heat conductivity, and good chemical stability. Therefore, AlN film has been used for BAW resonator and SAW device applications. However, the bandwidth of the AlN FBARs is not enough large for pratical use due to their low k value ($k^2 \cong 8$ %). Large piezoelectricity was recently reported in sputter-deposited ScAlN film[1)]. The d_{33} value of ScAlN film (≅ 25 pC/N) is 500 % of non-dope AlN[1)]. Our group reported the electromechanical coupling k value of ScAlN film and FBAR fabrication at first time [2,3)]. Several researchers also reported ScAlN film BAW resonators [4,5)], and they showed that the increase of Sc concentration induces the decrease of Q factor. On the other hand, Hashimoto *et al*. reported SAW resonator with high Q in high Sc concentration ScAlN film on SiC substrate [6)].

The k value of $Sc_xAl_{1-x}N$ films expected to show maximum near the phase boundary (x=0.5) [7)]. The piezoelectricity and elasticity of ScAlN film near the phase boundary in the GHz range are important.

In this study, the effect of Sc concentration on k_t, longitudinal wave velocity V_L and temperature coefficient of resonant frequency (TCF) in ScAlN films near the phase boundary were examined.

2. ScAlN film deposition

We fabricated $Sc_xAl_{1-x}N$ film (4 - 5 μm) by Sc ingot sputtering deposition[3)]. Sc ingots were placed on the Al target. Sc ingots and Al target were sputtered simultaneously, and ScAlN film was deposited on the substrate. By varying the amount of the introduced Sc ingots, Sc concentration in the films was adjusted. Fresh and good purity Sc metal ingot can be used for each fabrication in Sc ingot sputtering deposition. Silica glass (0.5 mm) was used as the substrate. Highly (0001) oriented Ti bottom electrode (100 – 200 nm) was deposited on the silica glass by using a DC sputtering.

Sc concentration of the films was evaluated by an energy dispersive X-ray spectrometry (JSM-7001FF, JEOL Ltd.).

A proportional relation was observed between the Sc concentration of the films and the amount of introduced Sc ingots.

Crystalline orientation and c-axis lattice length of the $Sc_xAl_{1-x}N$ films were examined by an X-ray diffraction (X-Pert Pro MRD, Philips). (0002) peak was observed in all samples. **Fig. 1 (a) and (b)** show (0002) rocking curve FWHM values and c-axis lattice length of $Sc_xAl_{1-x}N$ films, respectively. Almost the same FWHM values of (0002) rocking curve was observed in 0 < x < 0.39. The increase of Sc concentration in 0 < x < 0.3 induced the increase of c-axis lattice length. In contrast, $Sc_xAl_{1-x}N$ films in 0.35 < x < 0.41 exhibited the dramatic decrease of c-axis lattice length. The c-axis lattice length in x > 0.47 was much larger than that of non-dope AlN film.

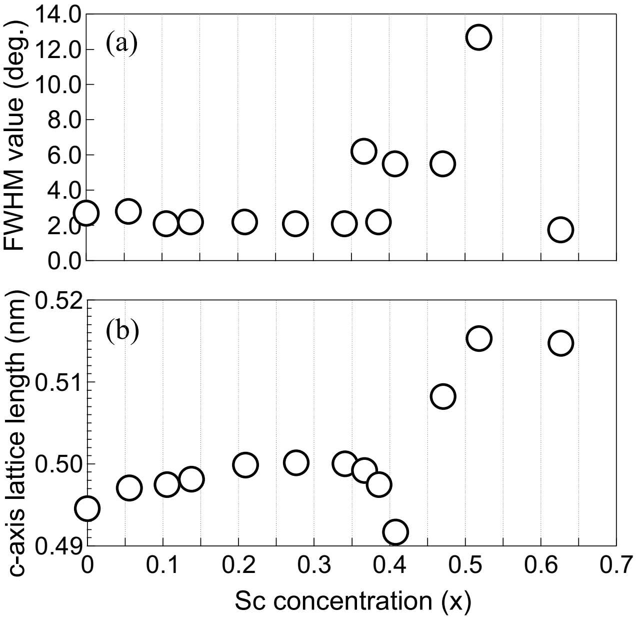

Fig. 1 (a) (0002) rocking curve FWHM value and (b) c-axis lattice length of the $Sc_xAl_{1-x}N$ films

3. k_t value and longitudinal wave velocity V_L of $Sc_xAl_{1-x}N$ films

In order to measure the longitudinal wave conversion loss of ScAlN films, the HBAR structures were fabricated by evaluating a Cu top electrode film (100 nm) on the samples. The conversion losses were measured by using a

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network analyzer (E5071C, Agilent Technologies). The k_t value and V_L of $Sc_xAl_{1-x}N$ films were determined from comparison of the measured conversion loss curve and the simulated one. The simulated conversion loss curves were obtained by using a Mason's equivalent circuit model. **Fig. 2 (a) and (b)** show k_t value and V_L of $Sc_xAl_{1-x}N$ films, respectively. The increase of Sc concentration in $0 < x < 0.41$ leaded the increase of the k_t value. $Sc_xAl_{1-x}N$ films in $x > 0.47$ exhibited the dramatic decrease of k_t value. A phase transition from a piezoelectric wurtzite phase to a non-piezoelectric cubic phase may be the reason of this decrease. The k_t value of $Sc_{0.41}Al_{0.59}N$ film near the phase boundary (≅ 0.35) was 1.3 times as high as that of non-dope AlN single crystal [8]. The increase of Sc concentration in $0 < x < 0.41$ leaded the decrease of V_L. The V_L of $Sc_{0.41}Al_{0.59}N$ film near the phase boundary (≅ 8000 m/s) was approximately 1.3 times as slow as that of non-dope AlN single crystal [8]. $Sc_xAl_{1-x}N$ films in $x > 0.47$ exhibited the increase of the V_L.

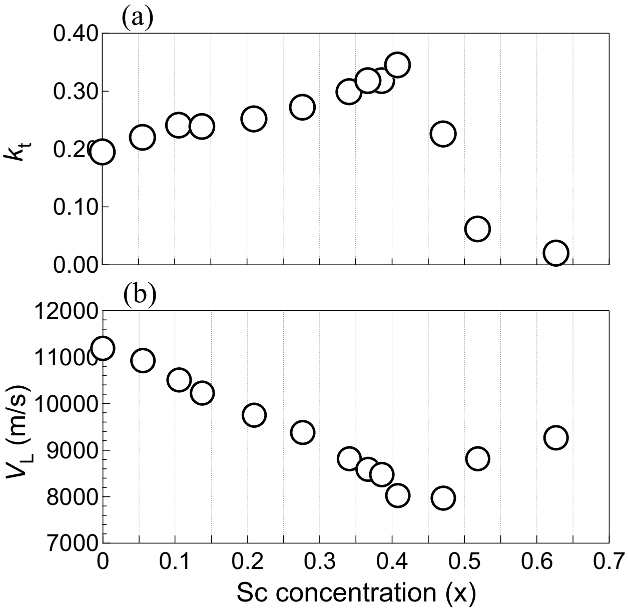

Fig. 2 (a) Electromechanical coupling k_t value and (b) longitudinal wave velocity V_L of the $Sc_xAl_{1-x}N$ films

4. Temperature coefficient of resonant frequency (TCF) in $Sc_xAl_{1-x}N$ films

The FBAR structures (with a Al top electrode (100 nm) / a $Sc_xAl_{1-x}N$ film / a Ti bottom electrode) were removed from the silica glass substrate using a scotch tape. Temperature characteristics of anti-resonant frequency of the FBARs were measured in 30 - 90 ºC at intervals of 15 ºC by using a network analyzer and a temperature control stage (Linkam, LK-600PM). Thickness extensional mode TCF values of $Sc_xAl_{1-x}N$ films were determined by fitting the plots with a linear function. **Fig. 3** shows TCF values of $Sc_xAl_{1-x}N$ films. TCF of $Sc_xAl_{1-x}N$ film in $0 < x < 0.21$ showed almost the same value (≅ -27 ppm / ºC), and this value was equal to that of pure AlN BAW resonator [9]. The increase of Sc concentration in $0.28 < x < 0.62$ leaded the gradual decrease of the TCF value. The TCF value in $Sc_{0.41}Al_{0.59}N$ film near the phase boundary was approximately -45 ppm / ºC.

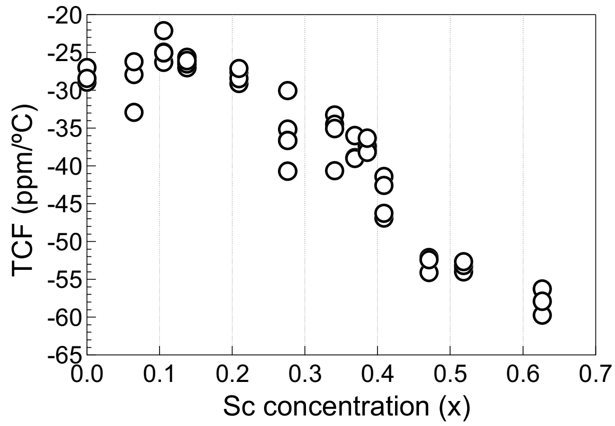

Fig. 3 TCF value of $Sc_xAl_{1-x}N$ films

5. Conclusion

The effect of Sc concentration in ScAlN films on electromechanical coupling k_t, GHz longitudinal wave velocity V_L and TCF value were examined. $Sc_{0.41}Al_{0.59}N$ film near the phase boundary shows the increase of k_t value (≅ 0.35), and the decrease of V_L (≅ 8000 m/s) and TCF value (≅ -45 ppm / ºC).

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