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A method to estimate k_t^2 of piezoelectric films from the change of lattice strain by XRD without removing substrate.

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***Abstract*— Electromechanical coupling coefficient k_t^2 is one of the important parameters to estimate performance of BAW filters. The resonance-antiresonance method according to IEEE standard is common method to determine k_t^2. However, this method requires a self-standing film structure (FBAR). In this study, we propose the k_t^2 estimation method for a film/substrate structure (HBAR). This method allows us to estimate k_t^2 for as grown wafers without removing substrates. The lattice strains of piezoelectric crystals are induced when electric field are applied. The strains can be measured by X-ray diffraction (XRD). Therefore, the k_t^2 of the film is expected to be indirectly determined by the use of piezoelectric equations. The values of k_t^2 determined by this method were compared with the resonance-antiresonance method and the conversion loss method.**

***Keywords—XRD, FBAR, lattice, piezoelectric thin film, electro mechanical coupling coefficient, ScAlN** (key words)*

I. Introduction

In previous study, the changes in lattice constant of a Rochelle salt under the external voltage were observed using X-ray diffraction. Vigness reported extractions of piezoelectric coefficient d_{33} and d_{14} by using the lattice strain [1]. Santos *et al.* reported the determination of all piezoelectric constants tensor of a bulk Rochelle salt crystal [2,3]. Time domain lattice strain analysis were even undertaken by a synchrotron radiation. However, there are a few facilities of synchrotron radiation around the world, i.e. Spring-8 (Japan), APS (America), and ESRF (France). On the other hand, powder X-ray diffractometer, XRD, is available in many laboratories. In this study, by using XRD, we propose a method to estimate k_t^2 of BAW piezoelectric films without removing substrate. k_t^2 is one of the most important parameter for determining the performance of the FBAR such as bandwidth and insertion loss. A resonance-antiresonance method is recommended for the k_t^2 determination of piezoelectric films, according to IEEE standard [4]. However, we need to prepare a self-standing film structure (FBAR) to use this method. It is convenient to determine the k_t^2 in film/substrate structure (HBAR) before preparing FBAR. Several methods are now available for HBAR structure such as the conversion loss method [5,6] and the resonant spectrum method [7].

II. Principle

To estimate static piezoelectricity of the film, we need to measure a mechanical strain. 2θ-ω scans can determine the distance between crystal planes in the thickness direction. The relationships between the lattice constant L and the scattering angle θ are given by (1).

$$L=n\lambda / 2 \sin \theta, \tag{1}$$

where λ is the wavelength of X-ray. Piezoelectric equations (d style) are given by

$$[S]=[s^E][T]+[d][E], \tag{2.1}$$

$$[D]=[d][T]+[\varepsilon^T][E], \tag{2.2}$$

where S, s^E, T, d, E, D, and ε^T is the strain, the elastic compliance (1/Pa), the stress (Pa), the piezoelectric coefficient (C/N), the electric field (V/m), the electric displacement (C/m^2), and the dielectric constant (F/m), respectively.

On the assumption that the stress $T=0$,

$$S=dE, \tag{3.1}$$

$$D=\varepsilon^{T}E, \tag{3.2}$$

are derived from (2.1), (2.2).

The piezoelectric coefficient d is determined by E and S from (3.1). A relationship between the d and k is given by (4).

$$k_t^2=d^2/s^{E}\varepsilon^{T} \tag{4}$$

As a result, the electromechanical coupling coefficient k_t^2 has been determined by the strain as a function of applied electric field.

III. Experiment

A. Fabrication of the ScAlN Resonator

Scandium aluminum nitride (ScAlN) films which has high piezoelectricity [8] was used for the experiment. ScAlN thin films with 6.1 μm thickness were grown on highly oriented Ti bottom electrode (200 nm)/silica glass (500 μm) substrate by RF magnetron sputtering. A schematic of the resonator consisting of Au/ ScAlN/ Ti/ silica glass substrate was shown in Fig. 1. Au was evaporated to the ScAlN film as a top electrode. The thickness of the film was determined by a stylus profiler (Kosaka laboratory ltd., Surfcoder SE-500). Also, Sc concentration of the films were obtained by an energy dispersive X-ray spectrometry, EDX (SHIMADZU, EDX-8000).

B. XRD Measurement

The degree of crystallization of the ScAlN thin film was measured by XRD (X'Pert PRO, PANalytical, Cu tube). The highly crystalline ScAlN film which has the ω scan rocking curve FWHM of 1.9 degree were observed. The measurement system of this study was shown in Fig. 1. A SMA connecter and variable DC supply were set to the ScAlN resonator in order to apply the external voltage. (0002) 2θ-ω XRD peaks of ScAlN were measured during the application of the DC voltage of -100 V to 150 V as shown in Fig. 2. The changes in the XRD patterns by the external voltage were observed.

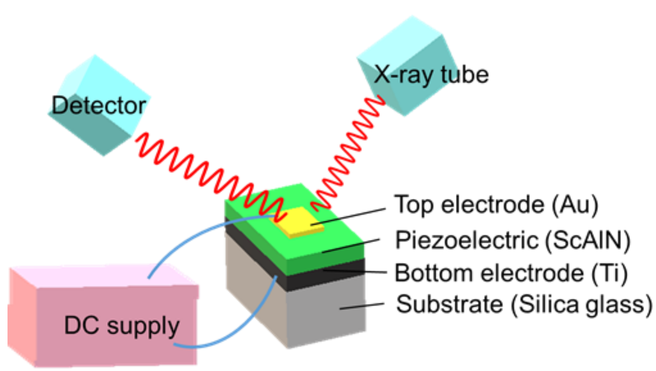

Fig. 1. The measurement system for the estimations of piezoelectricity by the change of lattice strain measured by XRD during the application of DC voltage.

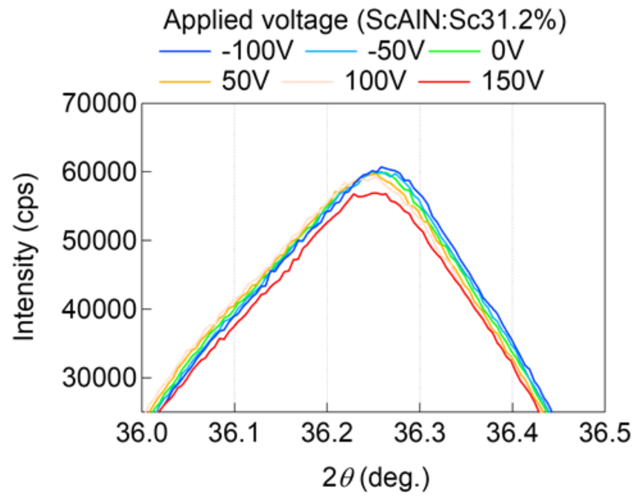

Fig. 2. (0002) XRD 2θ-ω peaks of the ScAlN film with the substrate. The DC voltage of -100 V to 150 V were applied to the ScalN films.

C. Estimation of electromechanical coupling coefficient

Using (1) and (5), the lattice strains S were obtained from the change of lattice constant L determined from the 2θ-ω XRD peaks. The peak maximums were determined by fitting a Gaussian function to each XRD pattern.

$$S=\left(L_{\mathrm{voltage}}-L_0\right)/\,L_0\ , \tag{5}$$

where L_{voltage} or L_0 are lattice constants when the voltage is applied or is not applied, respectively. The linear relationship between applied electric field and the lattice strain was observed in Fig. 3. The d_{33} was estimated by using the slope of this response without removing substrates by (3.1). Next, the electromechanical coupling coefficient k_t^2 were estimated by (4). The elastic stiffness c^E predicted by DFT [9] and the dielectric constants reported by Yanagitani *et al.* [10] were used. Here, the elastic stiffness c^E were converted to the elastic compliance s^E using (6). Next, using (4), the k_t^2 of the ScAlN film determined by present method was 17.7% with a HBAR structure. On the other hands, the k_t^2 determined by the conversion loss method [5.6] was 19.4%. Moreover, the FBAR structure were fabricated at same point of the measurement in the ScAlN film. The FBAR structures were fabricated by peeling the film off from the substrate by using a Scotch tape from the resonator. The k_t^2 of the ScAlN FBAR were determined to be 17.5% by the resonance-antiresonance method which IEEE standard has recommended as shown in Fig. 4.

$$s_{33}^{E}=\frac{c_{11}^{E}+c_{12}^{E}}{c_{33}^{E}(c_{11}^{E}+c_{12}^{E})-2{c_{13}^{E}}^{2}} \tag{6}$$

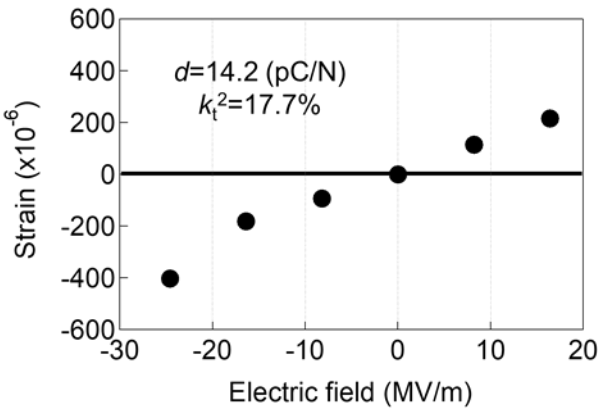

Fig. 3. The changes of the lattice strains of the ScAlN (Sc:31.2%) resonator without removing a substrate (HBAR).

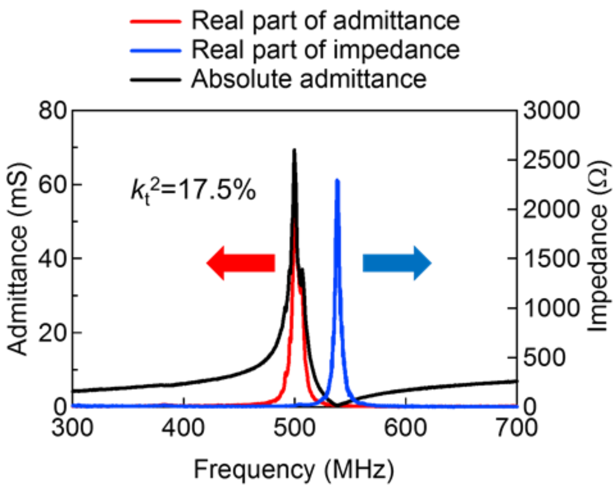

Fig. 4. Frequency characteristics of the real part of admittance and impedance of the ScAlN (Sc:31.2%) resonator with a free-standing film structure (FBAR).

IV. Effect of piezoelectricity

To verify that the change of XRD patterns was induced by piezoelectricity, AlN and ScAlN thin films were sputter-grown on a Ti bottom electrode/Si wafer substrate. The thicknesses of films were determined by a cross sectional SEM (JEOL, JSM-6500F) image. Additionally, Sc concentrations were obtained by a SEM-EDX. (0002) 2θ-ω XRD peaks of AlN (N-polar) and ScAlN (Al-polar) were measured during the application of the DC voltage of -50V to 50V or -150 V to 150 V as shown in Fig. 5. The sign of polarity of these films were determined by a press test as shown in Fig. 6. A positive and negative response indicates N-polarity and Al-polarity respectively. Also, the lattice strains S were obtained from the change of lattice constant L determined from the 2θ -ω XRD peaks as shown in Fig. 7. In Fig. 7, the slope of the ScAlN (Al-polar) response was opposite to AlN (N-polar) one. These opposite responses clearly indicate opposite signs of piezoelectric constants between AlN (N-polar) and ScAlN (Al-polar).

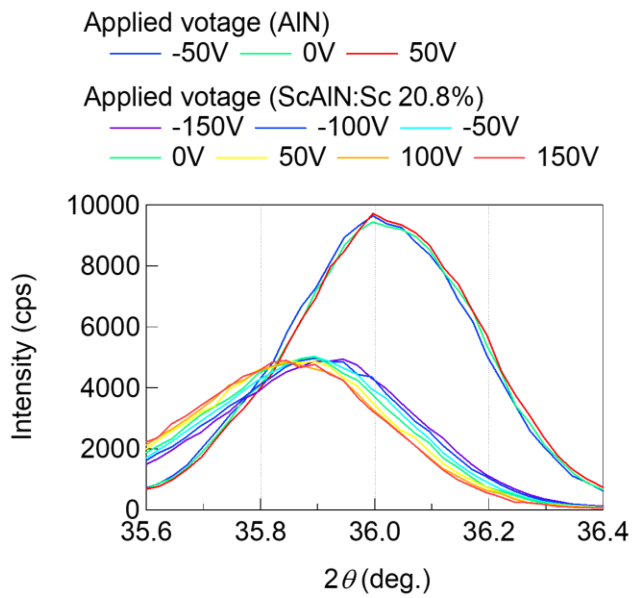

Fig. 5. (0002) XRD 2θ-ω peaks of the N-polar AlN and Al-polar ScAlN films which were applied the DC voltage of -50V to 50V or -150 V to 150 V.

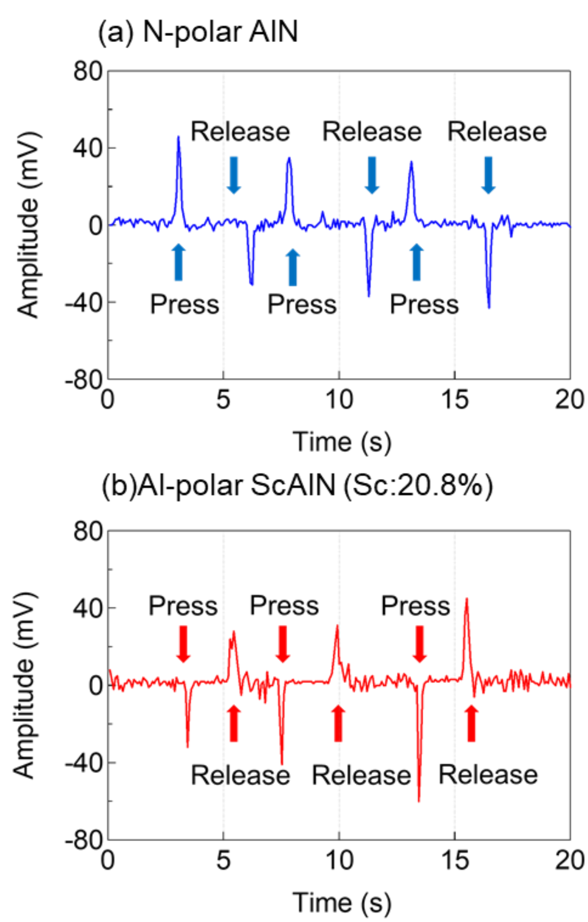

Fig. 6. Piezoelectric responses of (a)N-polar AlN and (b)Al-polar ScAlN by a press test.

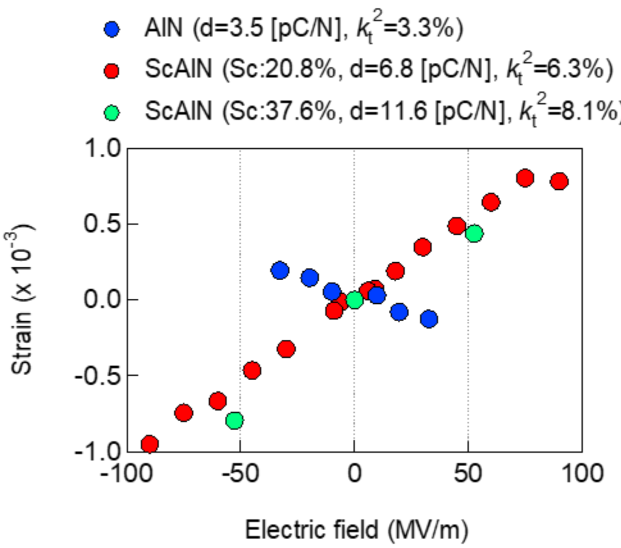

Fig. 7. The changes of the lattice strains of the AlN, ScAlN (Sc:20.8 %), and ScAlN (Sc:37.6%) resonators without removing the substrates (HBAR).

TABLE. I COMPARISON OF ELECTROMECHANICAL COUPLING COEFFICIENT OF THE FILMS WITH MULTIPLE METHOD

Sample	AlN	ScAlN (Sc:20.8%)	ScAlN (Sc:31.2%)	ScAlN (Sc:37.6%)
Thickness (μm)	1.06	1.06	6.1	0.94
d (pC/N)	3.48	6.84	14.2	11.6
s^E (1/Pa $\times$ 10^{-12})	2.93	4.61	6.28	7.96
$\varepsilon^T/\varepsilon_0$	13.1	18.2	20.5	23.6
k_t^2 (%) (This study)	3.32	6.29	17.7	8.09
k_t^2 (%) (Resonance-antiresonance)	---	---	17.5	---
k_t^2 (%) (Conversion loss)	---	---	19.4	---

V. CONCLUSION

We propose the k_t^2 estimation method for a film/substrate structure (HBAR) using XRD. The linear relationship between applied electric field and the lattice strain were observed. The piezoelectric coefficient d was estimated by using the slope of these responses without removing substrates. The k_t^2 values determined by other methods were shown in Table I for the comparison. The tendency of k_t^2 in the AlN and ScAlN films in the present method shows a good agreement with other methods such as the resonance -antiresonance method.

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