

# Correlation Between the Resonator Properties and Fourier Transform Infrared Spectra of Silicon Oxynitride Films for Surface Acoustic Wave Devices

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**Abstract**—In this paper, we discuss the temperature coefficient of frequency (TCF) and Q factor in the structure of  $\text{SiO}_x\text{N}_y/\text{LiTaO}_3$ . We studied the relationship of the TCF and Q factor with the optical properties of the  $\text{SiO}_x\text{N}_y$  films measured by Fourier transform infrared spectroscopy (FT-IR). We found that the Q factor of the device increased while TCF was decreased as the Si-O bond angle decreased in  $\text{SiO}_x\text{N}_y$  film. These results indicate that the Si-O atomic structure measured by FT-IR governs the device properties even when the N dopant is added.

**Keywords**—  $\text{SiO}_x\text{N}_y$  film, TCF, Q factor, FT-IR, Si-O bond

## I. INTRODUCTION

Surface Acoustic Wave (SAW) and Bulk Acoustic Wave (BAW) devices have been developed for the increasing number of the frequency bands. To meet the growing demand for high performance, thin amorphous dielectric films, silicon oxide ( $\text{SiO}_2$ ) and a silicon nitride ( $\text{Si}_3\text{N}_4$ ), were used to enhance the resonator performance.  $\text{SiO}_2$  thin film has a positive temperature coefficient of elasticity (TCE) [1], and it is used for improving the temperature coefficient of frequency (TCF) of the devices.  $\text{Si}_3\text{N}_4$  thin film is used for the passivation for the hermetic properties required [2].

In Refs. [3] and [4], the authors proposed to use a silicon oxynitride ( $\text{SiO}_x\text{N}_y$ ) thin film for the temperature-compensated surface acoustic wave devices (TC-SAW). This was proposed because the longitudinal-wave sound velocity of a  $\text{SiO}_x\text{N}_y$  thin film changed from 6,000 to 10,000 (m/s), respectively, and due to the nitrogen ratio  $N_y$  increasing [5]. Then, through experimentation, it was verified that the frequencies of the devices shifted higher in the structure of  $\text{SiO}_x\text{N}_y/\text{LiTaO}_3$  overlays as the nitrogen ratio  $N_y$  increasing. It was also shown that the Q factor of the device increased while TCF was decreased in this situation.

In this paper, the optical properties of the  $\text{SiO}_x\text{N}_y$  film are investigated, and then their correlation with the Q factor and TCF of the device is discussed. A series of SAW devices were fabricated using the  $\text{SiO}_x\text{N}_y/\text{Al}/\text{LiTaO}_3$  structure, and their

device performances were measured. The optical measurement was performed with the Fourier transform infrared spectroscopy (FT-IR) measurement [5], [6]. From the measurement results, we will discuss the mechanism of the Q factor and TCF with the nitrogen ratio  $N_y$ .

## II. FILM PREPARATION AND FT-IR MEASUREMENT

$\text{SiO}_x\text{N}_y$  films were deposited on (100) Si substrate by RF Sputtering in  $\text{Ar}/\text{O}_2/\text{N}_2$  atmosphere. By changing the  $\text{O}_2/\text{N}_2$  gas flow ratio from 0.25 to 0.40, we prepared three  $\text{SiO}_x\text{N}_y$  films which have different nitrogen ratio.  $\text{SiO}_2$  and  $\text{Si}_3\text{N}_4$  films were also deposited as a reference. Refractive index was measured by Ellipsometer and nitrogen ratio was measured by the X-ray photoelectron spectroscopy (XPS) method. As shown in Table.1, we prepared three  $\text{SiO}_x\text{N}_y$  films with the nitrogen ratio  $r=14.8, 24.4$  and  $43.3$  atomic %, respectively, in the same condition of the reference [3], [4].

The FT-IR measurements were performed for wave numbers between 400 and 1500  $\text{cm}^{-1}$  with a pitch of 1  $\text{cm}^{-1}$ . In  $\text{SiO}_x\text{N}_y$  films, the FT-IR spectra showed two main peaks around 470 and 1000  $\text{cm}^{-1}$  (Fig. 1). It is known that they are clarified with the direction of vibration of a rocking mode ( $\omega_1$ :  $\sim 450$   $\text{cm}^{-1}$ ) and a stretching mode ( $\omega_4$ :  $\sim 1070$   $\text{cm}^{-1}$ ) in the Si-O bonding [7], [8]. It is also known that Si-N bonding located at 890  $\text{cm}^{-1}$  [9]. It can be seen clearly in the sample C.

Table 1. Refractive index and N ratio  $r$  of prepared samples

Sample	Dielectric	Refractive index at 633nm	$y/(x+y)$ %
A	$\text{SiO}_x\text{N}_y$	1.558	13.8
B	$\text{SiO}_x\text{N}_y$	1.610	25.8
C	$\text{SiO}_x\text{N}_y$	1.712	42.1
Ref.	$\text{SiO}_2$	1.478	0
Ref.	SiN	2.019	100

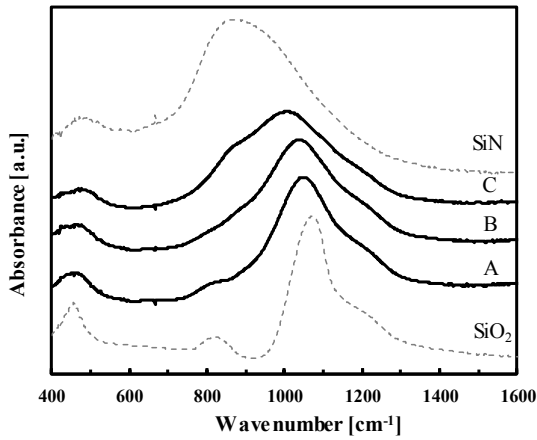


Fig.1 FT-IR spectra of the  $\text{SiO}_x\text{N}_y$  films

Table 2. FT-IR peaks of prepared samples

Sample	Dielectric	Rocking mode $\omega_1$	Stretching mode $\omega_4$
A	$\text{SiO}_x\text{N}_y$	461	1031
B	$\text{SiO}_x\text{N}_y$	467	997
C	$\text{SiO}_x\text{N}_y$	476	974
Ref.	$\text{SiO}_2$	457	1072
Ref.	$\text{SiN}$	492	890

Table 2 shows measured  $\omega_1$  and  $\omega_4$  of prepared samples. It is seen that  $\text{SiO}_x\text{N}_y$  films shows higher  $\omega_1$ , lower  $\omega_4$  and the wider full width of half maximum (FWHM)  $\Delta\omega_4$  of the absorption peaks as the nitrogen ratio  $N_y$  increasing.

### III. RESONATOR PROPERTIES

We fabricated one-port resonators by forming an IDT electrode with Al on a  $42^\circ\text{Y-X LiTaO}_3$  substrate. Then, the dielectric films of  $\text{SiO}_x\text{N}_y$  were deposited under the same conditions listed in Table 1 ( $\text{SiO}_2$  and  $\text{Si}_3\text{N}_4$  also deposited as a reference).

For a quality factor measurement, the Al film thickness were set to be  $h/\lambda_{\text{IDT}} = 0.085$  and  $0.077$ , and  $\text{SiO}_x\text{N}_y$  film thicknesses were set to be  $h/\lambda_{\text{IDT}} = 0.1$  and  $0.091$  ( $\lambda_{\text{IDT}}$  was set to be  $2.0$  and  $2.2\mu\text{m}$ , respectively). Figure 2 shows the input admittance  $Y$  of the one-port resonators. Table 3 shows the variation of estimated frequency and Q factor at the anti-resonance frequencies. It is seen that the SAW velocity  $V$  and the  $Q_a$  increased as the nitrogen ratio  $N_y$  increasing.

Figures. 3 and 4 show the correlation between  $Q_a$  and IR peak wavenumber. It is seen that  $Q_a$  increased as the  $\omega_1$  became higher, the  $\omega_4$  became lower. It is known that the Si-O bond angle is lower in the  $\text{SiO}_x\text{N}_y$  film when the  $\omega_1$  is higher and the  $\omega_4$  is lower [10]. These results indicate that the Q factor of the device is caused by the Si-O bond angle shift.

For the TCF measurement, the Al and  $\text{SiO}_x\text{N}_y$  film thicknesses were set to be  $h/\lambda_{\text{IDT}} = 0.04$  and  $h/\lambda_{\text{IDT}} = 0.25$  for a TCF measurement ( $\lambda_{\text{IDT}}$  was set to be  $2.0\mu\text{m}$ , respectively).

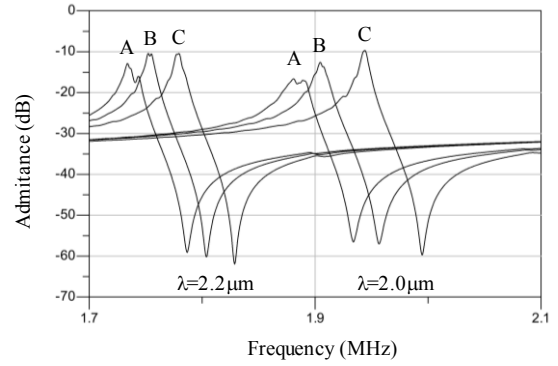


Fig.2 Measured Admittance of the SAW resonators

Table 3. Measured Q factor of prepared samples

Sample	Dielectric	$Q_a$ ( $\lambda=2.0\mu\text{m}$ )	$Q_a$ ( $\lambda=2.2\mu\text{m}$ )
A	$\text{SiO}_x\text{N}_y$	334	428
B	$\text{SiO}_x\text{N}_y$	342	463
C	$\text{SiO}_x\text{N}_y$	455	615
Ref.	$\text{SiO}_2$	187	193
Ref.	$\text{SiN}$	640	581

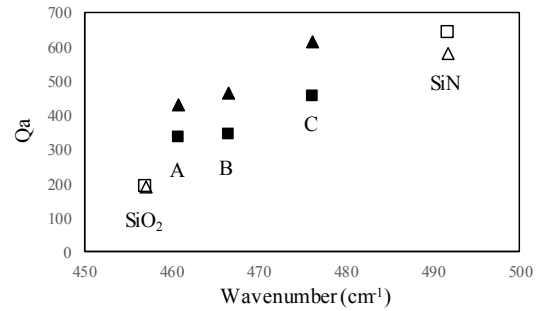


Fig.3 Relationship between  $\omega_1$  and  $Q_a$

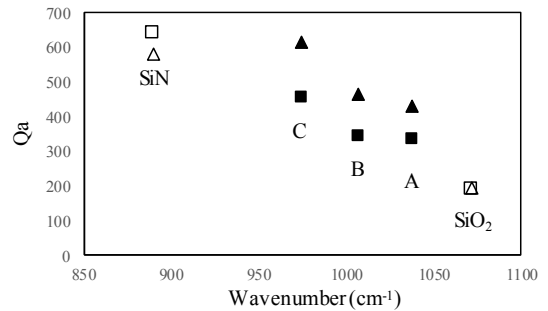


Fig.4 Relationship between  $\omega_4$  and  $Q_a$

Table 4 shows the variation of estimated TCF. It is seen that the TCF decreased as the nitrogen ratio  $N_y$  increasing.

Figures. 5 and 6 show the correlation between TCF and IR peak wavenumber. It is seen that TCF increased as the  $\omega_1$  became lower, the  $\omega_4$  became higher. These results well agree

Table. 4. Measured TCF of prepared samples

Sample	N ratio	TCF [ppm/°C]
A	14.8	2.0
B	24.4	-12.5
C	43.3	-20.5
Ref.	0	-28
Ref.	100	-40

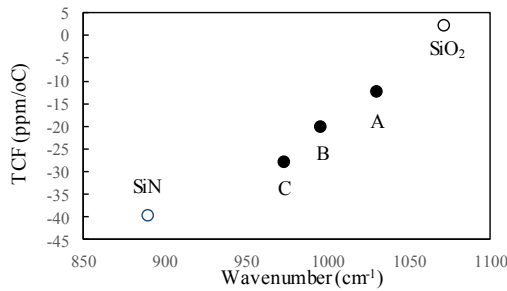


Fig.5 Relationship between  $\omega_1$  and  $Qa$

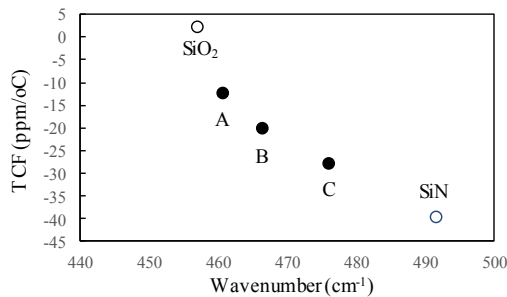


Fig.6 Relationship between  $\omega_4$  and  $Qa$

with the previous results [5], indicating that the TCF of the device with  $\text{SiO}_x\text{N}_y$  film is also principally governed by the change in the Si–O bond angle.

#### IV. SUMMARY

This paper discusses the optical properties of the  $\text{SiO}_x\text{N}_y$  film for the temperature compensated SAW devices using the

$\text{SiO}_x\text{N}_y/\text{LiTaO}_3$  structure. From the FT-IR measurement, it was experimentally verified that the Q factor of the device increased while TCF was decreased as the peak frequency  $\omega_4$  of Si-O bond decreased and its peak width  $\Delta\omega_4$  increased by the nitrogen ratio  $N_y$  increasing.

It is known that the Si-O bond angle is around  $144^\circ$  [8] and Si-N bond angle is around  $120^\circ$  [11]. In the situation, Si-O bond angle shift smaller and the distribution of the bond angle is larger. The smaller Si-O bond angle leads to increase and less space to move. In this situation, the sound velocity increased and decrease the temperature coefficient of velocity (TCV) [12]. These results indicated that the tradeoff between the the Q factor and TCF is governed by the bonding structure in the  $\text{SiO}_x\text{N}_y$  film.

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