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

Abstract—In this paper, we discuss the temperature coefficient of frequency (TCF) and Q factor in the structure of SiO$_x$N$_y$/LiTaO$_3$. We studied the relationship of the TCF and Q factor with the optical properties of the SiO$_x$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 SiO$_x$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—SiO$_x$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 (SiO$_2$) and a silicon nitride (Si$_3$N$_4$), were used to enhance the resonator performance. 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. Si$_3$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 (SiO$_x$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 SiO$_x$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 SiO$_x$N$_y$/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 SiO$_x$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 SiO$_x$N$_y$/Al/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

SiO$_x$N$_y$ films were deposited on (100) Si substrate by RF sputtering in Ar/O$_2$/N$_2$ atmosphere. By changing the O$_2$/N$_2$ gas flow ratio from 0.25 to 0.40, we prepared three SiO$_x$N$_y$ films which have different nitrogen ratio. SiO$_2$ and Si$_3$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 method. As shown in Table 1, we prepared three SiO$_x$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 cm$^{-1}$ with a pitch of 1 cm$^{-1}$. In SiO$_x$N$_y$ films, the FT-IR spectra showed two main peaks around 470 and 1000 cm$^{-1}$ (Fig. 1). It is known that they are clarified with the direction of vibration of a rocking mode ($\omega_r$: ~450 cm$^{-1}$) and a stretching mode ($\omega_s$: ~1070 cm$^{-1}$) in the Si-O bonding [7], [8]. It is also known that Si-N bonding located at 890 cm$^{-1}$ [9]. It can be seen clearly in the sample C.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Dielectric</th>
<th>Refractive index at 633nm</th>
<th>y/(x+y) %</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>SiO$_x$N$_y$</td>
<td>1.558</td>
<td>13.8</td>
</tr>
<tr>
<td>B</td>
<td>SiO$_x$N$_y$</td>
<td>1.610</td>
<td>25.8</td>
</tr>
<tr>
<td>C</td>
<td>SiO$_x$N$_y$</td>
<td>1.712</td>
<td>42.1</td>
</tr>
<tr>
<td>Ref.</td>
<td>SiO$_2$</td>
<td>1.478</td>
<td>0</td>
</tr>
<tr>
<td>Ref.</td>
<td>SiN</td>
<td>2.019</td>
<td>100</td>
</tr>
</tbody>
</table>

Table 1. Refractive index and N ratio of prepared samples
Table 2 shows measured $\omega_1$ and $\omega_4$ of prepared samples. It is seen that SiO$_x$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 Y–X LiTaO$_3$ substrate. Then, the dielectric films of SiO$_x$N$_y$ were deposited under the same conditions listed in Table 1 (SiO$_2$ and Si$_3$N$_4$ also deposited as a reference).

For a quality factor measurement, the Al film thickness were set to be $h/\lambda_{IDT} = 0.085$ and 0.077, and SiO$_x$N$_y$ film thicknesses were set to be $h/\lambda_{IDT} = 0.1$ and 0.091 ($\lambda_{IDT}$ was set to be 2.0 and 2.2 μm, 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 SiO$_x$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 SiO$_x$N$_y$ film thicknesses were set to be $h/\lambda_{IDT} = 0.04$ and $h/\lambda_{IDT} = 0.25$ for a TCF measurement ($\lambda_{IDT}$ was set to be 2.0 μm, respectively).

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

For the TCF measurement, the Al and SiO$_x$N$_y$ film thicknesses were set to be $h/\lambda_{IDT} = 0.04$ and $h/\lambda_{IDT} = 0.25$ for a TCF measurement ($\lambda_{IDT}$ was set to be 2.0 μm, respectively).
with the previous results [5], indicating that the TCF of the device with SiO$_x$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 SiO$_x$N$_y$ film for the temperature compensated SAW devices using the SiO$_x$N$_y$/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° [8] and Si-N bond angle is around 120° [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 SiO$_x$N$_y$ film.

REFERENCES