Temperature Characteristics of SH-type Acoustic Waves in a Rotated *Y*-cut $LiTaO_3$ Thin Plate

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***Abstract* — The SH (shear horizontal) -type surface acoustic wave (SH-SAW) on 36° *Y-X* $LiTaO_3$ has a high electromechanical coupling factor k^2 of about 0.047 and a comparatively low temperature coefficient of delay (TCD) of about 32 ppm/°C. The temperature coefficient of the relevant shear stiffness constant for the SH-SAW on 36° *Y-X* $LiTaO_3$ changes its sign if the electric field in the substrate could be thoroughly short-circuited. Therefore the TCD of the 0-th SH-type plate wave propagating in a very thin 36° *Y-X* $LiTaO_3$ plate with surface electrodes would be expected to be lower due to the electric-field short-circuiting by the surface electrodes. This paper reports theoretical calculations and experiments on the 0-th SH-type plate wave propagating along the *X*-axis in a thin θ°-rotated *Y*-cut $LiTaO_3$ plate. It is shown that the TCD becomes zero at θ=20.1° and 67.1° for the case of an infinitesimally thin plate. Between these two cut angles, the SH-type plate wave has a negative TCD. In the 36°*Y-X* finite-thickness plate with surface electrodes on its both sides, the TCD becomes zero at a normalized plate thickness of $h/\lambda = 0.236$ (h: plate thickness, λ: wavelength), where the electromechanical coupling factor k^2 is as high as 0.18. If a ferroelectric inversion layer is formed in the plate, the plate thickness at which TCD becomes zero can be increased. Some experimental results on the 0-th SH-type plate wave in thin 36° *Y-X* $LiTaO_3$ plates are presented and compared with the theoretical calculation.**

Keywords – zero temperature coefficient of delay; shear-horizontal wave; coupling factor; lithium tantalate; resonator filter

I. Introduction

It is well known that the leaky surface acoustic wave (LSAW) on rotated *Y-X* $LiTaO_3$ substrate reduces to a shear-horizontal (SH) type surface acoustic wave (SAW) at a rotation angle of about 36° [1]. The rotated *Y*-cut $LiTaO_3$ substrates with cut angle from 36° to 42° are in practical use in various SAW devices such as RF-SAW filters in cellphones. The SH-SAW on 36° *Y-X* $LiTaO_3$ has a high electromechanical coupling factor k^2 of about 0.047 and relatively small temperature coefficient of delay (TCD) of about 32 ppm/°C. In recent years, however, there is a growing need for lower TCD devices.

The temperature coefficient of delay for the SH-SAW propagating along the *X*-axis on the 36°-rotated *Y*-cut $LiTaO_3$ substrate with free surface is about 45.3 ppm/°C. If the electric field in the substrate could be thoroughly short-circuited, the TCD is expected to become about −12.9 ppm/°C because the elastic stiffness c^D is replaced by c^E of which temperature coefficient is of opposite sign to that of c^D [2]. Hence, when the substrate surface is metalized, the TCD of the SH-SAW falls between 45.3 and −12.9 ppm/°C, that is about 32 ppm/°C, because the electric field is short-circuited only at the surface [1]. If the rotated *Y*-cut $LiTaO_3$ substrate with surface electrodes is made much thinner than the wavelength, the SH-SAW reduces to the 0-th mode SH-type plate wave (henceforth referred to as the "SH-wave"), and the TCD is expected to approach −12.9 ppm/°C because the electric field in the thin plate is short-circuited by the surface electrodes.

In this paper, the SH-wave in a thin θ° *Y-X* $LiTaO_3$ plate is theoretically analyzed by taking the plate thickness into account and it is demonstrated that the SH-wave has a vanishing TCD and a substantially high coupling factor k^2 of about 18% at a plate thickness-to-wavelength ratio. Experimental results on SH-wave resonators utilizing reflection at the plate edges [3] are also presented and compared with the theoretical ones.

II. Temperature Coefficient of Delay

In the following calculations, the material constants of $LiTaO_3$ reported by Smith *et al.* [4] are used. The temperature coefficient of delay for the fast shear bulk wave propagating along the *X*-axis in the $LiTaO_3$ crystal, which has a displacement vector almost the same as that of the SH-SAW on 36° *Y-X* substrates, is given by:

$$\mathrm{TCD} = \alpha_{11} - \frac{1}{V}\cdot\frac{\partial V}{\partial T} \tag{1}$$

$$= -2.05\times10^{-6} - \frac{1}{2}\cdot\frac{1}{c_{55}^D}\cdot\frac{\partial c_{55}^D}{\partial T} \tag{2}$$

where α_{11} is the thermal expansion coefficient in the crystalline *X* direction, V is the phase velocity, T is the temperature, and c_{55}^D is the elastic stiffness at constant electric displacement in the coordinate system obtained by a rotation of the crystallographic coordinates (X, Y, Z) by the angle of 36° about the X-axis. As $-(1/c_{55}^{D})\cdot(\partial c_{55}^{D}/\partial T)$ is about 94.6 ppm/°C, TCD is about 45.3 ppm/°C, which is almost equal to that of the SH-SAW on the free surface [1]. If the electric field in the crystal could be thoroughly short-circuited, c_{55}^{D} in (2) should be replaced by the elastic stiffness at constant electric field c_{55}^{E}. As $-(1/c_{55}^{E})\cdot(\partial c_{55}^{E}/\partial T)$ is about −21.7 ppm/°C, TCD is about −12.9 ppm/°C. This shows that the temperature characteristics are improved if the electric field could be short-circuited. Hence, if the rotated Y-cut $LiTaO_3$ substrate is made much thinner than the wavelength, the SH-SAW reduces to the 0-th mode SH-wave and the TCD is expected to approach −12.9 ppm/°C because the electric-field in the plate is short circuited by the surface electrodes.

III. THEORETICAL ANALYSIS

A. SH-wave in an Infinitesimally Thin Plate

Fig. 1 shows the 0-th SH-wave propagating along the X-axis in a thin θ°-rotated Y-cut $LiTaO_3$ plate with metallized surfaces. If the plate thickness h is assumed to be infinitesimally thin, the equation of motion for the SH-wave can be written as:

$$\rho\frac{\partial^2 u_3}{\partial t^2}=\frac{\partial T_5}{\partial x_1}, \tag{3}$$

where ρ is the density, u_3 is the displacement, and T_5 is the shear stress given by:

$$T_5=\left(c_{55}^{E}-\frac{c_{56}^{E\,2}}{c_{66}^{E}}\right)\frac{\partial u_3}{\partial x_1}\equiv c_{55}^{\prime E}\frac{\partial u_3}{\partial x_1}, \tag{4}$$

where c_{55}, c_{56}, and c_{66} are the elastic stiffness constants in the plate coordinate system (x_1, x_2, x_3). The equation of motion can be rewritten as follows by substituting (4) into (3):

$$\rho\frac{\partial^2 u_3}{\partial t^2}=c_{55}^{\prime E}\frac{\partial^2 u_3}{\partial x_1{}^2}. \tag{5}$$

From (5), the phase velocity V_m can be given as:

$$V_m=\sqrt{c_{55}^{\prime E}/\rho}. \tag{6}$$

From (6), the TCD for the SH-wave can be expressed as:

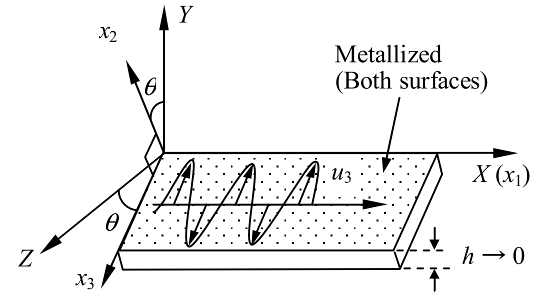

Figure 1. SH-wave in a infinitesimally thin rotated Y-X $LiTaO_3$ plate.

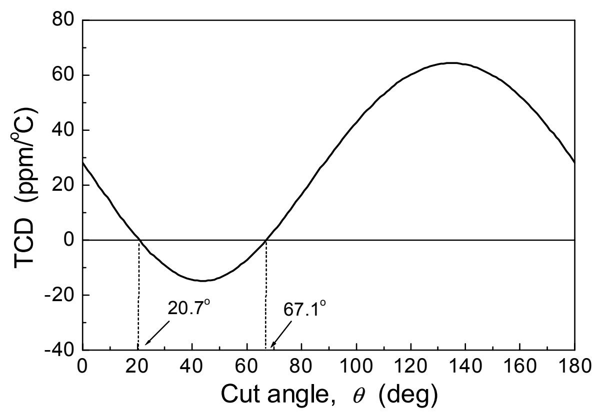

Figure 2. Temperature coefficient of delay for the SH-wave in a infinitesimally thin θ°-rotated Y-X $LiTaO_3$ plate as a function of θ.

$$\begin{aligned}\mathrm{TCD}&=\alpha_{11}-\frac{1}{2}\left(\frac{1}{c_{55}^{\prime E}}\frac{\partial c_{55}^{\prime E}}{\partial T}-\frac{1}{\rho}\frac{\partial\rho}{\partial T}\right)\\&=-2.05\times10^{-6}-\frac{1}{2}\left(\frac{1}{c_{55}^{\prime E}}\frac{\partial c_{55}^{\prime E}}{\partial T}\right).\end{aligned} \tag{7}$$

Fig. 2 shows the TCD calculated by (7) as a function of cut angle θ. It is found that TCD becomes zero at θ= 20.7° and 67.1°. Between these two cut angles, TCD is negative and has a minimum value of −14.7 ppm/°C at θ = 43.8°.

B. SH-wave in a Finite Thickness Plate

Consider a plate with a finite thickness here. As the thickness increases, the SH-wave in a rotated Y-X $LiTaO_3$ plate with surface electrodes changes to a combined mode of two SH-SAWs propagating on the top and bottom surfaces of the plate. Therefore the TCD of the SH-wave seems to increase from −12.9 ppm/°C at h = 0 to 32 ppm/°C at h = ∞, which corresponds to the TCD of the SH-SAW. To study the effect of the plate thickness on the TCD of the SH-wave, the theoretical analysis was carried out with considering the finite plate thickness h.

Fig. 3 shows the calculated phase velocity of the SH-wave as a function of normalized plate thickness h/λ (h: plate thickness, λ: wavelength). The dotted, solid, and broken curves indicate the phase velocities for the electrically-free surfaces case, the metallized surfaces case, and the one-side metallized surface case, respectively. In Fig. 3, the phase velocity of the SH-wave in the plate with free surfaces approaches that for the plate with metallized surfaces as the plate thickness approaches zero. This means that the electric field in the plate is substantially short-circuited even if there is no electrode on the plate surface. This is because the internal electric displacement normal to the plate surface becomes zero when the plate is very thin, and therefore the external electric displacement also becomes zero.

Fig. 4 shows the electromechanical coupling factor k^2 of the SH-wave calculated by the following equation:

$$k^2 = 2\frac{V_f - V_m}{V_f}. \tag{8}$$

With increasing h/λ, k^2 increases from zero at $h/\lambda = 0$ and takes a large maximum of about 19% around $h/\lambda = 0.08$.

Fig. 5 shows the calculated TCD. The TCD for the free surface case is negative at $h/\lambda = 0$, but it sharply increases with h/λ. The TCD for the one-side metallized surface case increases gradually with h/λ, and it becomes zero at a normalized plate thickness h/λ of 0.128, where the coupling factor k^2 is as high as 0.17. When the plate has electrodes on its both surfaces, the TCD becomes zero at h/λ=0.236, where k^2 is as high as about 0.18.

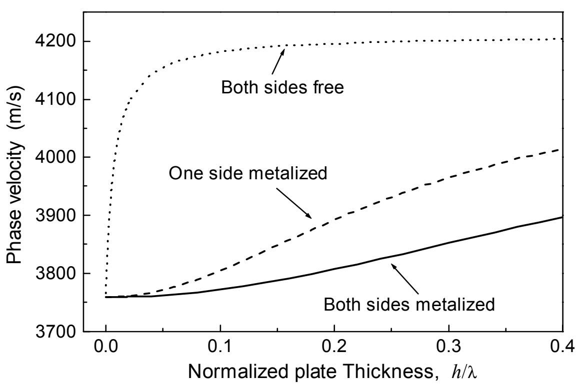

Figure 3. Phase velocity of the SH-wave in the 36° *Y-X* $LiTaO_3$ plate as a function of normalized plate thickness h/λ (h: plate thickness, λ: wavelength).

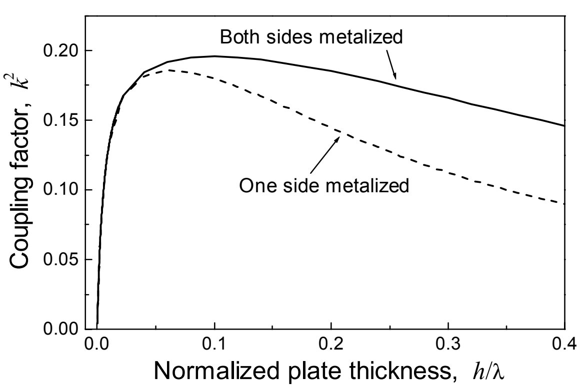

Figure 4. Coupling factor k^2 of the SH-wave in the 36° *Y-X* $LiTaO_3$ plate as a function of normalized plate thickness h/λ.

C. *Effect of Ferroelectric Inversion Layer*

From the above-mentioned results, the $LiTaO_3$ plate must be very thin compared with the wavelength λ to achieve a zero TCD. Therefore the SH-wave in thin $LiTaO_3$ plates seems suitable for the application in relatively low frequency devices. If the plate thickness for zero TCD can be increased, however, the frequency range suitable for applications of the SH-wave will be extended toward higher frequencies.

It is well known that a domain inversion takes place at the negative surface of proton-exchanged $LiTaO_3$ plates with heat treatment near the Curie temperature [5], [6]. In such a plate with an inversion layer, the domain boundary possesses a sort of electric-filed short-circuiting effect [2] and it would improve the temperature characteristics of the SH-wave [2].

To examine the effect of a ferroelectric inversion layer, the SH-wave in a thin θ °-rotated *Y-X* $LiTaO_3$ plate with an inversion layer of thickness h_I was also theoretically analyzed. Fig. 6 shows the calculated TCD and the coupling factor k^2 for

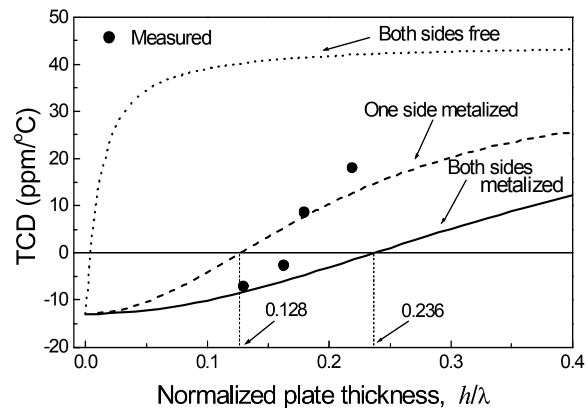

Figure 5. Temperature coefficient of delay for the SH-wave in the 36° *Y-X* $LiTaO_3$ plate as a function of normalized plate thickness h/λ. Measured values for the one-side metallized surface case are indicated as dots.

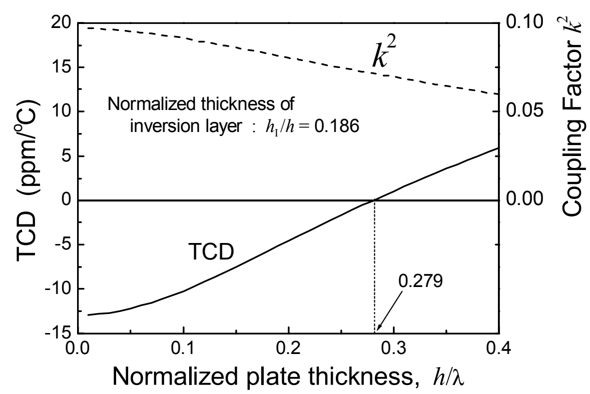

Figure 6. TCD and coupling factor k^2 of the SH-wave in a 36° *Y-X* $LiTaO_3$ plate with an inversion layer on the top surface side and an electrode on the bottom surface as a function of normalized plate thickness h/λ.

the 36° *Y-X* plate with an inversion layer on the top surface side and an electrode on the bottom surface. It is seen that the TCD becomes zero at $h/\lambda = 0.279$, which is about 2.2 times as large as the thickness of the plate with no inversion layer for zero TCD.

IV. EXPERIMENTS

To experimentally confirm the theoretical results, SH-wave resonators utilizing SH-wave reflection at the plate edges [3], schematically shown in Fig. 7, were fabricated using 36° *Y-X* $LiTaO_3$ plates about 70 μm thick. Each resonator had a 7-finger-pair IDT with an electrode period L of 320, 390, 430, or 540 μm and an overlap length W of 4 mm on the top surface of the plate, while the bottom surface was electrically free. Fig. 8 shows the measured electrical admittance of the resonator whose electrode period L is 430 μm. The difference of the admittance level between the resonance frequency and anti-resonance frequency is as large as 100 dB. The resonance frequency at which the phase of the admittance was zero was measured with an impedance analyzer over the temperature range from 0°C to 60°C. Figure 9 shows the temperature dependence of the resonance frequency of this resonator. The TCD at 25°C is evaluated to be about –2.78 ppm/°C, which is very small as compared with the TCD of the SH-SAW, that is, about 32 ppm/°C. The measured TCD values of four resonators are plotted as dots in Fig. 5, by substituting h/L with h/λ. It can be seen that the measured TCD follows the same trend as the theoretical curve.

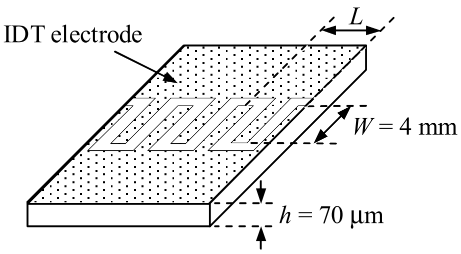

Figure 7. Resonators utilizing SH-wave reflection at the plate edges of a 36° *Y-X* $LiTaO_3$ plate.

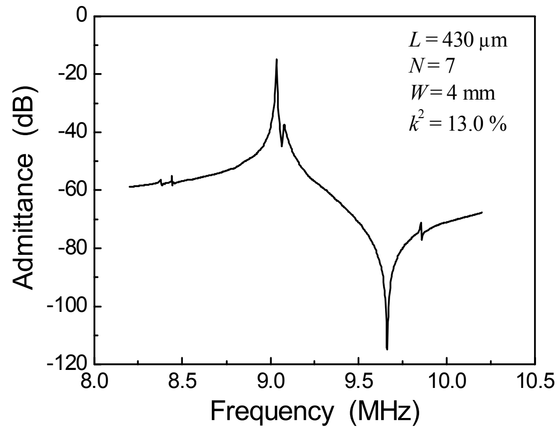

Figure 8. Measured electrical admittance of the resonator with the electrode period L of 430 μm.

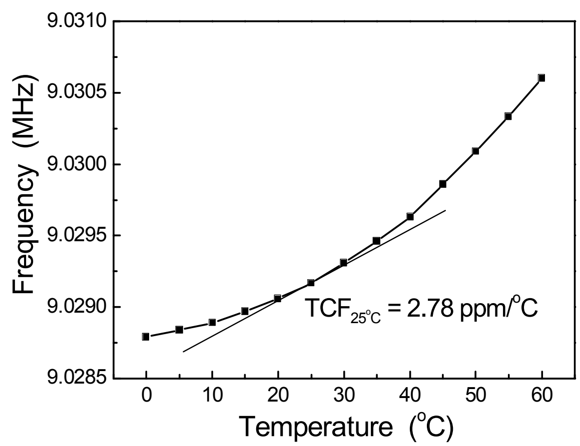

Figure 9. Temperature dependence of the resonance frequency of an SH-wave resonator.

V. CONCLUSION

The temperature coefficient of delay for the 0-th SH-wave in a thin θ°-rotated *Y-X* $LiTaO_3$ plate has been studied. It has been shown theoretically that the TCD of the SH-wave in the infinitesimally thin plate with surface electrodes becomes zero at $\theta = 20.7°$ and 67.1°, and it is negative between these two cut angles. Considering the effect of the plate thickness h, the TCD of the SH-wave in the 36° *Y-X* $LiTaO_3$ plate has been calculated to become zero at a certain thickness, where k^2 is as high as about 0.18. The experimental results on the SH-wave resonators utilizing reflection at the plate edges have shown that the TCD values follow the same trend as the theoretical calculations and can be made zero by controlling a normalized plate thickness h/λ. The 0-th SH-wave in a thin rotated *Y-X* $LiTaO_3$ plate would be promising for relatively low frequency devices such as IF filters for the digital televisions.

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