Effect of Polarity of $LiTaO_3$ and Quartz on Hetro Acoustic Layer Surface Acoustic Wave Properties

Michio Kadota
Department of Robotics, Graduate School of Engineering
Tohoku University
Sendai, Miyagi, Japan
mkadota@tohoku.ac.jp

Shuji Tanaka
Department of Robotics, Graduate School of Engineering
Tohoku University
Sendai, Miyagi, Japan
mems@tohoku.ac.jp

***Abstract*— We developed advanced surface acoustic wave (SAW) devices so-called Hetero Acoustic Layer (HAL) SAW devices by combining thin $LiTaO_3$ (LT) and rot.Y90ºX quartz (Qz). High impedance (*Z*) ratio over 80 dB, near-zero TCF and spurious-free characteristics up to 14 GHz have been achieved. In the previous study, we theoretically investigated the performance dependence on the polarity of LT and Qz. Bandwidth (BW) and *Z* ratio of HAL SAW resonators with four combinations of the polarity of 10-50ºYX LT and 42º45'Y90ºX Qz, +LT−/ +Qz−, +LT−/ −Qz, −LT+/ +Qz−, and −LT+/ −Qz, were calculated. The combinations of −LT+/ +Qz− and −LT+/ −Qz+ exhibit wider BW and higher *Z* ratio than +LT−/ +Qz− and +LT−/ −Qz+. In this study, we experimentally confirmed the BW and the *Z* ratio dependence on the polarity of 42ºYX LT and 60ºY90ºX Qz. In addition, we discuss the combinations of LT and Qz crystallographically equivalent to the combination.**

Keywords—HAL SAW, polarity, combination of Euler angle, $LiTaO_3$, quartz, impedance ratio, bandwidth

I. INTRODUCTION

Surface acoustic wave (SAW) or bulk acoustic wave (BAW) filters have been widely used in mobile phones [1][2]. In recent years, with the increasing prevalence of smartphones, the frequency spectrum has become crowded. So, their filters are strongly required to have a steeper passband and a lower temperature coefficient of frequency (TCF). SAW resonators with a high impedance (*Z*) ratio or high Q factor and low TCF are crucial for fabricating ladder filters with desirable properties.

Previously, we reported Hetero Acoustic Layer (HAL) SAW resonators combined thin $LiTaO_3$ (LT) and rotated (rot.) Y90ºX quartz (Qz) [3][4]. We fabricated a HAL SAW resonator composed of a Cu interdigital transducer (IDT) and 205ºYX thin LT/ 60ºY90ºX Qz substrate, i.e. IDT/ –LT+/ +Qz– structure as described below. It showed a suitable bandwidth (BW) of 4.5% and a high impedance (*Z*) ratio of 84 dB, which was 7% wider BW and 33 dB higher *Z* ratio than a standard SAW device composed of 42ºYX LT.

In this paper, the BW and *Z* ratio are defined as $(f_a - f_r)/ f_r$ and $20{\cdot}\log(Z_a/ Z_r)$, respectively (f_r and f_a are resonant and anti-resonant frequencies, and Z_r and Z_a are resonant and anti-resonant impedances, respectively.

This research and development work was partly supported by the SCOPE #JP225002001.

In addition to the high *Z* ratio, the LT/ Qz HAL SAW also possesses near-zero TCF and spurious-free characteristics up to 14 GHz, making it useful for carrier aggregation systems [3][4]. SAW resonators composed of an LT thin film/ SiO_2 film/ Si substrate structure also exhibit a high *Z* ratio of 81 dB, a high Bode Q of 4,200, and a low TCF in the 2 GHz range [5][6].

Nakamura *et al.* reported that the polarity of a $LiNbO_3$ (LN) structure on an IDT/c-axis oriented ZnO piezoelectric thin film (c ZnO) / 128ºYX LN substrate theoretically affects the electro-mechanical coupling factor [7]. The coupling factor on the c ZnO/ +LN plane is five times larger than that on the c ZnO/ –LN plane, with a normalized ZnO film thickness of 0.04λ (λ: wavelength). It was also reported that the coupling factors of the c ZnO film combined with a YX LN substrate, which lacks piezoelectric polarity, were influenced by the polarity of the ZnO film [8]. The coupling factor of the positive c ZnO film/ YX LN is larger than that of the negative c ZnO/ YX LN [8]. Hence, in the combination of a piezoelectric thin film and a piezoelectric substrate, each polarity affects the coupling factor.

In a previous study, we theoretically investigated the effect of the polarity of 10-50ºYX LT and 42º45'Y90ºX Qz on the properties of four different combinations of each polarity, and reported the polarity of the LT influences the properties [4]. In this paper, we fabricated HAL SAW resonators by combining the positive and negative planes of 42ºYX LTs and 60ºY90ºX Qzs and measured their frequency characteristics, and discuss not only their polarity but also combinations of LT and Qz that are crystallographically equivalent to rot.YX LT/ rot.Y90ºX Qz.

II. HAL SAW COMBINING 42ºYX LT AND 60ºY90ºX QZ

A. Simulation

A rot.YX LT/ rot.Y90X Qz HAL SAW has a wider BW and higher *Z* ratio than rot.YX LT/ rot.YX Qz. So, rot.YX LT/ rot.Y90X Qz HAL SAW is discussed. LT and LN crystals have piezoelectric properties by polarization. Negative and positive charges are generated on the positive and negative polarization voltage planes, respectively. These planes are referred to as the negative and positive planes., respectively.

On the other hand, Qz has positive and negative planes geometrically but lacks piezoelectric polarity since Qz crystal is non-polarized. Euler angles of the positive and negative planes of a 42ºYX LT are (0º, 312º, ψ), which is equivalent to (0º, –48º, ψ), and (0º, 132º, ψ), respectively. A 42ºYX LT with

(0º, 312º, 0º) surface and (0º, 132º, 0º) back plane is represented as +(42ºYX LT)–. Similarly, 60ºY90ºX Qz with (0º, 330º, 90º) surface of +plane and (0º, 150º, 90º) back plane of –plane is represented as +(60ºY90ºX Qz)–.

We simulated and fabricated four combinations of polarization using 42ºY LT and 60ºY90ºX Qz, (a) −LT+/ −Qz+, (b) −LT+/ +Qz−, (c) +LT−/ −Qz+, and (d) +LT−/ +Qz−. For example, "−LT+/ +Qz−" means that the positive plane of LT and the positive plane of Qz are bonded and that the IDT is on the −LT plane.

Figs. 1 and 2 show calculated BWs and *Z* ratios of the four combinations, respectively, at Al IDT thickness of 0.12λ and LT thickness of 0.05λ to 0.6λ. (a) –LT+/ –Qz+ and (b) –LT+/ +Qz– exhibit the same characteristics, just as (c) +LT–/ –Qz+ and (d) +LT–/ +Qz– do. Hereinafter, the polarity of Qz is omitted, and –LT+/ Qz or +LT–/ Qz is used. –LT+/ Qz have wider BWs and higher *Z* ratios compared to +LT–/ Qz. The characteristics depend on LT polarity but not on quartz polarity. The same results are observed for the combinations of 10-50°YX LT and 42º45'Y90ºX Qz in our previous paper [4].

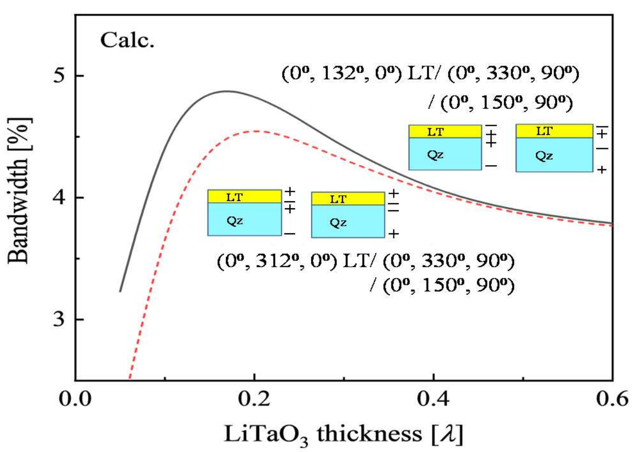

Fig. 1 Simulated BWs of four combinations of 42ºYX LT and 60ºY90ºX Qz as a function of LT thickness.

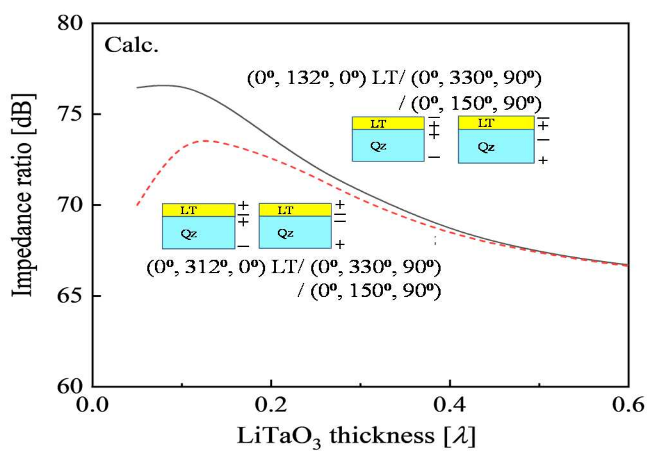

Fig. 2 Simulated *Z* ratios of of four combinations of 42ºYX LT and 60ºY90ºX Qz as a function of LT thickness.

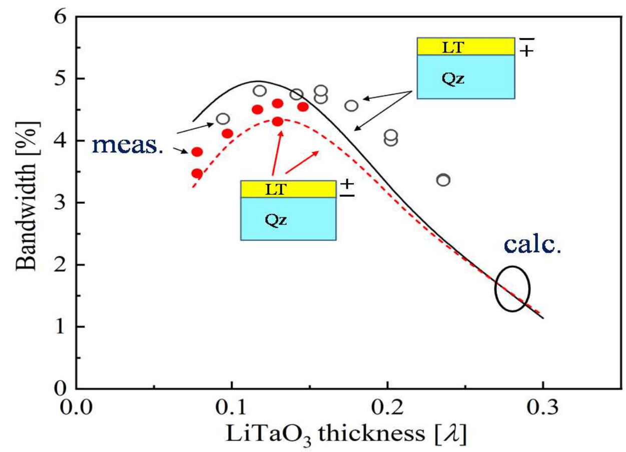

Fig. 3 Measured and simulated BWs of (0º, 132º, 0º) LT(–LT+)/ 60ºY90ºX Qz and (0º, 312º, 0º) LT(+LT–)/ 60ºY90ºX Qz (white circles and black solid line, and red circles and broken line, respectively).

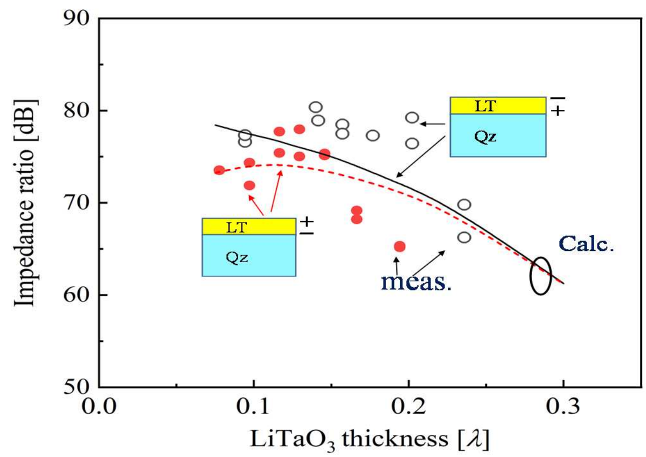

Fig. 4 Measured and simulated *Z* ratios of (0º, 132º, 0º) LT(–LT+)/ 60ºY90ºX Qz and (0º, 312º, 0º) LT(+LT–)/ 60ºY90ºX Qz (white circles and black solid line, and red circles and broken line, respectively).

B. Fabrication and measurement

LT with a mirror surfaces of (0°, 132°, 0°) or (0°, 312°, 0°) was bonded to 60°Y90°X Qz. The former is –LT+/ Qz and the latter is +LT–/ Qz. The LTs were polished to 0.3-0.66 μm in thickness. The LT thickness variation is due to the limited controllability of polishing. 0.4 μm thick Al IDTs with λ of 2.4-6 μm, an aperture of 30-60λ, and 48-80 IDT pairs, and a grating reflector of 30 fingers at each side of the IDT were fabricated on them.

Figs. 3 and 4 show the simulated and measured BWs and *Z* ratios of HAL SAW resonators in terms of LT normalized thicknesses, respectively. It should be noted that the normalized Al thickness varies depending on the wavelength. White and red circles represent the measured data for −LT+/ Qz and +LT−/ Qz, respectively. Black solid and red broken lines show the simulated BWs and *Z* ratios for −LT+/ Qz and +LT−/ Qz, respectively. They were calculated at a constant Al thickness of 0.4 μm. Therefore, each Al thickness normalized by wavelength is different. Since the average measured BWs and *Z* ratios are larger than the simulated ones, the simulated BWs and Z ratios have been scaled up slightly to approximate the measured values in Figs. 3 and 4. The data show some dispersion probably due to LT variation and fabrication imperfection. However, the measured BWs and *Z* ratios are in general agreement with the simulated ones. At the LT thicknesses of 0.1-0.15λ, the measured results show that –LT+/ Qz has BWs about 5-11% wider and *Z* ratios 3-6 dB higher compared to +LT−/ Qz. This result well agrees with the theoretical prediction shown in Figs. 1 and 2.

III. Crystallographically Equivalent Combination

Four types of Euler angles of (0º, 132º, 0º), (0º, 132º, 180º), (0º, 312º, 0º) and (0º, 312º, 180º) LT have the same velocity as 42ºYX LT and are acoustically equivalent. Additionally, four types of Euler angles of (0º, 150º, 90º), (0º, 330º, 90º), (0º, 150º, 270º), and (0º, 330º', 270º) Qz are also acoustically equivalent as 60ºY90ºX Qz. Consequently, there are 16 combinations of Euler angles for 42ºYX LT and 60ºY90ºX Qz.

Table I shows the simulated characteristics of the 16 combinations using 0.12λ thick Al IDT and 0.1λ thick LT. The 8 combinations in Group A are crystallographically equivalent to the (0º, 132º, 0º) LT/ (0º, 150º, 90º) Qz and (0º, 132º, 0º) LT/ (0º, 330º, 90º) Qz shown in Figs. 1 and 2. Eight combinations in Group B also to (0º, 312º, 0º) LT/ (0º, 150º, 90º) Qz and (0º, 312º, 0º) LT/ (0º, 330º, 90º) Qz. Group A exhibits a 21% wider BW and a 3 dB higher *Z* ratio than Group B. Even when using +LT–/ Qz combination, the combinations in Group A demonstrate better properties. Finally, the following combinations show desirable properties.

(0º, 90 to 270º, 0º) LT (–LT+) / (0º, θ_{Qz}, 90º) Qz
(0º, 90 to 270º, 0º) LT (–LT+) / (0º, θ_{Qz}, 270º) Qz
(0º, 90 to 270º, 180º) LT (–LT+) / (0º, θ_{Qz}, 90º) Qz
(0º, 90 to 270º, 180º) LT (–LT+) / (0º, θ_{Qz}, 270º) Qz
(0º, –90 to 90º, 0º) LT (+LT–) / (0º, θ_{Qz}, 90º) Qz
(0º, –90 to 90º, 0º) LT (+LT–) / (0º, θ_{Qz}, 270º) Qz
(0º, –90 to 90º, 180º) LT (+LT–) / (0º, θ_{Qz}, 90º) Qz
(0º, –90 to 90º, 180º) LT (+LT–) / (0º, θ_{Qz}, 270º) Qz

Table I Simulated characteristics of the 16 combinations using 42ºYX LN and 60ºY90ºX Qz.

	LT(φ,θ,ψ)			Polarity	Qz (φ,θ,ψ)			Polarity	V_r	V_a	BW	*Z* ratio
	φ	θ	ψ	LT	φ	θ	ψ	Qz	m/s	m/s	(%)	(dB)
A	0º	132º	0º	−LT+	0º	150º	90º	−Qz+	3588	3752	4.6	76.9
						330º		+Qz−				
			180º			150º	270º	−Qz+				
						330º		+Qz−				
		312º	0º	+LT−		150º	270º	−Qz+				
						330º		+Qz−				
			180º			150º	90º	−Qz+				
						330º		+Qz−				
B	0º	132º	0º	−LT+	0º	150º	270º	−Qz+	3581	3719	3.8	73.9
						330º		+Qz−				
			180º			150º	90º	−Qz+				
						330º		+Qz−				
		312º	0º	+LT−		150º	90º	−Qz+				
						330º		+Qz−				
			180º			150º	270º	−Qz+				
						330º		+Qz−				

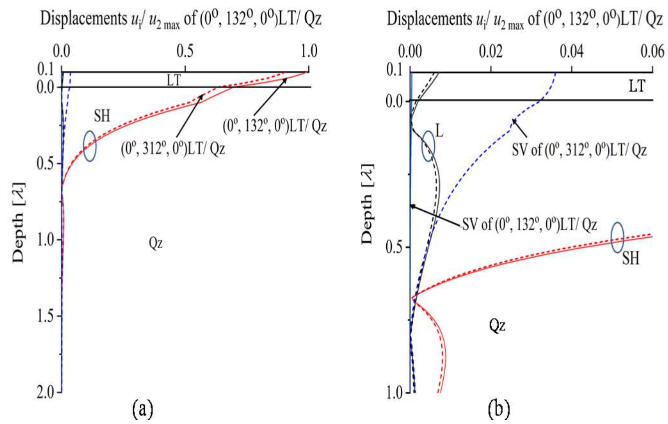

Fig. 5 (a) Simulated distributions of absolute values of displacement on (0º, 132º, 0º) LT(–LT+) and (0º, 312º, 0º) LT(+LT–)/ 60ºY90ºX Qzs by solid and broken lines, respectively. (b) enlargement of (a).

IV. Distributions of Displacement

We discuss the differences in properties between HAL SAW resonators composed of two different combinations. Fig. 5 shows the distributions of absolute values of displacement on (0º, 132º, 0º) LT(–LT+)/ 60ºY90ºX Qz and (0º, 312º, 0º) LT(+LT–)/ 60ºY90ºX Qz, at an Al thickness of 0.12λ and a LT thickness of 0.1λ. Fig. 5 (b) is an enlarged view of Fig. 5 (a). Longitudinal (L), SH, and shear vertical (SV) components are shown by black, red, and blue lines, respectively. The solid and broken lines show the displacements of (0º, 132º, 0º) LT(–LT+) and (0º, 312º, 0º) LT(+LT–)/ 60ºY90ºX Qz, respectively. Their displacements are normalized by the maximum displacement (u_2 component: shear horizontal (SH)) on the surface of (0º, 132º, 0º) LT(–LT+)/ 60ºY90ºX Qz.

The former SH component is larger than the latter on the surface as shown in Fig. 5 (a). As shown Fig. 5 (b), the SV component differs between the two structures, with the former having almost zero SV component, while the latter has a significant SV component. The previous reports said that SAW resonators with a high concentration of displacements could achieve a high *Z* ratio [4][5]. This disparity in the concentration of displacement in the SV component might be the reason behind wider bandwidth (BW) and higher Z ratio observed in the former structure.

V. Combination of LN and Qz

Figs. 6 and 7 show simulated BWs and *Z* ratios of 2 combinations, (–LN+/ +Qz–) and (+LN–/ +Qz–), consisting of (0º, 101º, 0º) LN/ (0º, 341º, 90º) Qz and (0º, 281º, 0º) LN/ (0º, 341º, 90º) Qz, respectively, as a function of LN thickness. The combination of –LN+/ +Qz– shows a wider BW and higher *Z* ratio compared to the combinations of +LN–/ +Qz– and +LN– / –Qz+.

Table II shows the simulated properties of the 16 combinations using 11ºYX LN and 70ºY90ºX Qz with a 0.07λ thick Cu IDT and 0.1λ thick LN. Among them, 8 combinations crystallographically equivalent to (0º, 101º, 0º) LN (–LN+) / (0º, 341º, 90º) Qz (+Qz–) have wider BWs and higher *Z* ratios compared to them on (0º, 281º, 0º) LN (+LN–)/ (0º, 341º, 90º) Qz (+Qz–) as well as combinations of LT/ Qz.

The effect of combinations of LN polarity and Qz Euler angle is smaller compared to the effect of LT/ Qz. LT/ Qz provides a 21% wider BW and 3 dB higher *Z* ratio in the simulation, whereas –LN+/ Qz provides a half of them, with 11% wider and 1.6 dB higher compared to +LN–/ Qz.

VI. Conclusion

The HAL SAW properties of the four polarization combinations using 42ºY LT and 60ºY90ºX Qz were simulated. Their characteristics depend on the LT polarity but not on the Qz polarity. The fabricated HAL SAW resonators using (0º, 132º, 0º) LT (–LT+)/ (0º, 330º, 90º) Qz exhibited a 5-11% wider BW and a 3-6 dB higher *Z* ratio at 0.1-0.15λ thick LT compared to the (0º, 312º, 0) LT (+LT–)/ (0º, 330º, 90º) Qz device. The results are in good agreement with the simulated characteristics. There are 8 combinations equivalent to (0º, 132º, 0º) LT (–LT+) / (0º, 330º, 90º) Qz, all exhibiting the same propertie Similarly, there are also 8 combinations equivalent to (0º, 312 0) LT (+LT–)/ (0º, 330º, 90º) Qz, also all exhibiting the sam properties. Although the combinations of LN and Qz were als studied, their effect was relatively small compared to LT/ Qz approximately by a half. Therefore, selecting the optima combination of LT and Qz is crucial for achieving desirabl properties in LT/ Qz HAL SAWs.

References

[1] M. Kadota, "Development of substrate structures and processes fo practical applications of various surface acoustic wave devices," Jpn. . Appl. Phys. 44, p. 4285, 2005.

[2] R. Ruby, P. Bradley, D. Clark, D. Feld, T. Jamneala and Kun Wang "Acoustic FBAR for filters, duplexers and front end modules," in Proc Int. IEEE MTT-S Microwave Symp., 2, 2004, p. 931.

[3] M. Kadota, Y. Ishii, T. Shimatsu, M. Uomoto, and S. Tanaka," Suprious Free, Near-Zero-TCF Hetero Acoustic Layer (HAL) SAW Resonators Using $LiTaO_3$ Thin Plate on Quartz," in Proc. Int. IEEE Ultrason. Symp., 6J-2, 2018.

[4] M. Kadota, Y. Ishii, and S. Tanaka, "Surface Acoustic Wave Resonators of Hetero Acoustic Layer (HAL) Structure Using Lithium Tantalate and Quartz," IEEE trans. Ultrason. Ferroelec. Freq. Contr., p. 1955, 2020.

[5] T. Takai, H. Iwamoto, Y. Takamine, H. Yamazaki, T. Fuyutsume, H. Kyoya, T. Nakao, H. Kando, M. Hiramoto, T. Toi, M. Koshino, and N. Nakajima, "High-Performance SAW Resonator on New Multilayered Substrate Using $LiTaO_3$ Crystal," IEEE Trans. Ultrason. Ferroelectr. Freq. Contr. 64, p. 1382, 2017.

[6] T. Takai, H. Iwamoto, Y. Takamine, T. Fuyutsume, T. Nakao, M. Hiramoto, T. Toi, and M. Koshino, "High-Performance SAW Resonator with Simplified $LiTaO_3/SiO_2$ Double Layer Structure on Si Substrate," IEEE Trans. Ultrason. Ferroelectr. Freq. Contr. 66, p. 1006, 2019.

[7] K. Nakamura and T. Hanaoka, Propagation Characteristics of Surface Acoustic Waves in $ZnO/LiNbO_3$ Structures," Jpn. J. Appl. Phys. 32, Part 1, p. 2333, 1993.

[8] M. Kadota and K. Minami, "Surface Acoustic Wave Characteristics on ZnO/YZ·$LiNbO_3$ Structure and Their Application to Elastic Convolver," Jpn. J. Appl. Phys. 34, Part 1, p. 2698, 1995.

[9] M. Kadota, Y. Ishii, and S. Tanaka, "Capability of $LiTaO_3$/ Quartz HAL SAW Resonators Confirmed by Simulation and Measurement," in Proc. int. IEEE Freq. Contr. Symp., 2019, MoAT1-1.

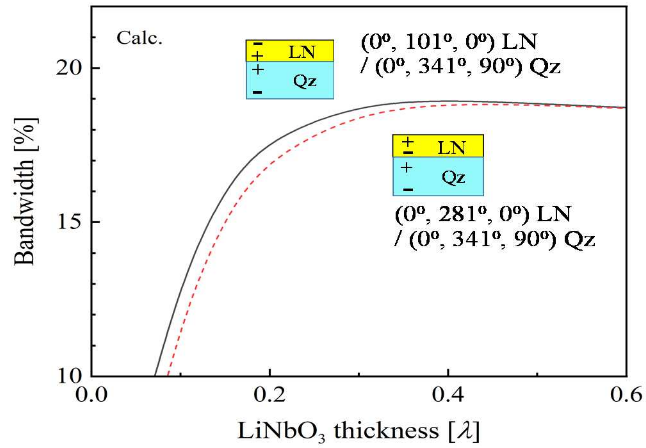

Fig. 6 Simulated W of -LN+/ +Qz and +LN-/ +Qz- using 11ºYX LN and 70ºY90ºX Qz as a function of LN thickness.

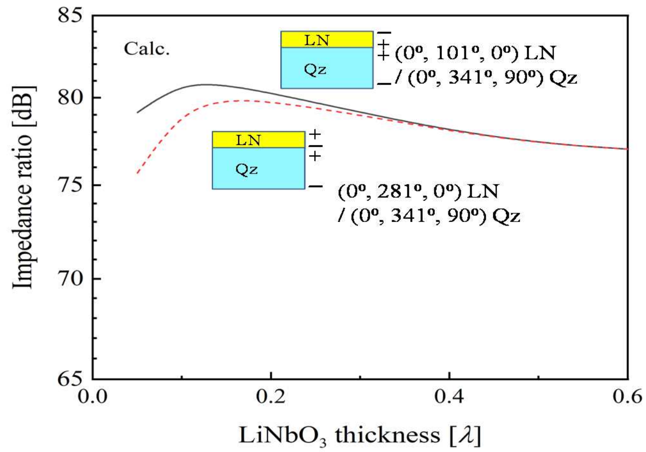

Fig. 7 Simulated *Z* ratios of –LN+/ +Qz– and +LN–/ +Qz– using 11ºYX LN and 70ºY90ºX Qz as a function of LN thickness.

Table II Simulated characteristics of the 16 combinations using 11ºYX LN and 70ºY90ºX Qz.

	LN(φ,θ,ψ)			Polarity	Quartz (φ,θ,ψ)			Polarity	V_r	V_a	BW	Z ratio
	φ	θ	ψ	LN	φ	θ	ψ	Qz	m/s	m/s	(%)	(dB)
C	0º	101º	0º	−LN+	0º	160º	90º	−Qz+	2874	3252	13.1	80.9
						340º		+Qz−				
			180º			160º	270º	−Qz+				
						340º		+Qz−				
		281º	0º	+LN−		160º	270º	−Qz+				
						340º		+Qz−				
			180º			160º	90º	−Qz+				
						340º		+Qz−				
D	0º	101º	0º	−LN+	0º	160º	270º	−Qz+	2876	3216	11.8	79.3
						340º		+Qz−				
			180º			160º	90º	−Qz+				
						340º		+Qz−				
		281º	0º	+LN−		160º	90º	−Qz+				
						340º		+Qz−				
			180º			160º	270º	−Qz+				
						340º		+Qz−				