Optimal orientations of LiTaO3 for application in plate mode resonators
Natalya F. Naumenko

Citation: Journal of Applied Physics 118, 034505 (2015); doi: 10.1063/1.4926871
View online: http://dx.doi.org/10.1063/1.4926871
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/118/3?ver=pdfcov
Published by the AIP Publishing

Articles you may be interested in
Direct and converse magnetoelectric effects in Metglas/LiNbO3/Metglas trilayers

Acousto-optic interaction of leaky surface acoustic waves in Y-cut LiTaO3 crystals

Anisotropic acousto-optic diffraction by leaky wave radiation in Z X - Li Nb O 3

Line-focus acoustic microscopy measurements of acoustic properties of LiTaO3 crystal plates with an inversion layer
J. Appl. Phys. 81, 6616 (1997); 10.1063/1.365201

Photoluminescence of LiTaO 3 :Pr
Optimal orientations of LiTaO$_3$ for application in plate mode resonators

Natalya F. Naumenko

Acousto-Optical Research Center, National University of Science and Technology “MISIS,”
Moscow 119049, Russia

(Received 22 May 2015; accepted 5 July 2015; published online 15 July 2015)

Optimal cuts of LiTaO$_3$ for application in plate mode resonators were found via rigorous numerical investigations of zero- and higher-order plate modes propagating parallel or normal to the X-axis in rotated Y-cuts of LiTaO$_3$; the plates were tested with a periodic metal grating on top of the plate and metal electrode present or absent on the plate bottom. In some cuts, high electromechanical coupling coefficients up to 20% could be combined with low or even zero temperature coefficients of frequency (TCF). Other cuts ensured moderate coupling of 12%–14% and low TCF in addition to high velocity of a higher-order plate mode up to 20000 m/s. Metallization of a plate bottom helped to enhance coupling of certain modes. Interaction of a plate mode with electrodes of an interdigital transducer or with periodic metal gratings used for its excitation and reflection in resonators is illustrated by examples of dispersion plots. The nature of the analyzed modes was studied via visualization of the mechanical displacements accompanying wave propagation. © 2015 AIP Publishing LLC [http://dx.doi.org/10.1063/1.4926871]

I. INTRODUCTION

Acoustic modes propagating in thin plates of piezoelectric crystals (membranes) are characterized by wide-ranging velocities dependent on plate thickness. Such plate modes can be efficiently excited by interdigital transducers (IDTs) and utilized in resonators.\(^1\) Compared to surface acoustic wave (SAW) resonators, which are widely used today in mobile phones and other communication devices, plate mode resonators enable higher frequencies and wider bandwidths due to potentially very high velocities and larger electromechanical coupling coefficients typical of bulk acoustic waves (BAWs). Extremely high velocities exceeding 15 000 m/s required for gigahertz radio frequency (RF) resonators can be achieved in very thin plates. Fabrication of such plates with parallel faces is a challenge today, but the advantages of obtaining high-velocity modes with moderate or high electromechanical coupling and simplicity in their excitation using common IDTs are strong reasons for the rapid development of such technologies. Recently, thin plates of LiNbO$_3$ (LN) were successfully applied in high-frequency resonators with the operating frequency exceeding 5 GHz (Ref. 2) and ultra-wideband resonators for low-frequency tunable filters.\(^3\) These advances were achieved due to rapid progress in fabrication technologies and optimization of LN orientations to provide maximum electromechanical coupling coefficients for zero-order shear horizontally polarized (SH$_0$) mode and first-order quasi-anti-symmetric mode ($qA_1$).

In LiTaO$_3$ (LT), plate modes have not been as thoroughly investigated, although in addition to high velocities and high coupling up to 20%, low or zero temperature coefficients of frequency (TCF) can be obtained for plate modes propagating in this material.\(^4,5\) LT orientations with low TCF could be used in wideband resonators with improved temperature characteristics. The main objective of this paper is to find and investigate the optimal orientations in which plate modes demonstrate high coupling and low or zero TCF combined, if possible, with high velocity. This goal is achieved via rigorous numerical investigation of plate modes propagating under a periodic Al grating in rotated Y-cuts of LT.

II. METHODS OF INVESTIGATION

The typical structures of plate mode resonators are shown in Figure 1: IDTs and periodic metal gratings with a pitch $p$ are used for lateral excitation and reflection of plate modes in a thin piezoelectric membrane, which rests on two silicon bars. The technological process of fabricating such structures was previously described.\(^6\) A metal film (electrode) added to the bottom of a plate helps to enhance electromechanical coupling of certain modes. Therefore, the search for optimal orientations with maximum coupling was

![Figure 1](https://via.placeholder.com/150)

**FIG. 1.** Two structures of plate mode resonators: (a) without additional films; (b) with an aluminum electrode at the bottom of the LT plate.
performed for the structures both without such an electrode (Figure 1(a)) and with it (Figure 1(b)). For simplicity, an optimization procedure was performed for plate modes propagating under an infinite periodic metal grating. The electrical parameters of finite-length resonators could be simulated using well known techniques with the determined plate mode characteristics as initial data.

The advanced numerical technique SDA-FEM-SDA, which was originally developed for SAW resonators and later successfully applied to the investigation of Lamb waves and other plate modes in AlN, AlN/SiO2, and LN, was used to calculate the admittance functions of the LT resonators. This technique combines finite element modeling (FEM) analysis of the IDT electrodes with spectral-domain analysis (SDA) of the upper half-space (air) and the lower half-space (piezoelectric plate of finite thickness with or without a metal film at the bottom and air half-space below). The plate mode velocities $V_R = 2\pi f_R$ and $V_A = 2\pi f_A$ were found at resonant $f_R$ and anti-resonant $f_A$ frequencies extracted from the admittance function, and the electromechanical coupling $k^2$ of each mode was estimated from the frequency shift between $f_R$ and $f_A$:

$$k^2 = \frac{\pi f_R}{2 f_A} \tan^{-1} \left( \frac{\pi f_R}{2 f_A} \right).$$

Accurate values for velocities $V_R$ and $V_A$ found at and around room temperature $T_0 = 25^\circ$ C enabled the determination of the TCF

$$TCF_{RA} = \frac{[V_{RA}(t_0 + \Delta) - V_{RA}(t_0 - \Delta)]}{V_{RA}(t_0)}/2^\circ - \alpha',$$

where $\alpha'$ is the thermal expansion coefficient estimated for the analyzed propagation direction using the reported constants of LT crystal. In practice, the finite length of an LT plate confined between LT/Si structures may influence the temperature behavior of plate modes, but this minor effect was ignored in the search for optimal cuts for plate mode resonators.

Similar to SAW, plate modes propagating under a periodic metal grating with fixed thickness and geometry of electrodes can be characterized by the Coupling-Of-Mode (COM) parameters, which are further used in resonator design procedures. COM parameters include velocity, electromechanical coupling, and reflection coefficient. The reflection coefficient can be determined via analysis of plate mode dispersion in a periodic grating. The calculated dispersion of plate modes revealed the influence of a thin metal electrode at the bottom of an LT plate on the plate mode behavior. The numerical technique based on the method of Rational Approximation of Admittance (RAA) was used to simulate dispersion of plate modes in open-circuit (OC) and short-circuit (SC) gratings.

To optimize LT cuts for resonators based on different plate modes, the characteristics of these modes were investigated as functions of LT thickness and cut angles. The nature of the analyzed modes is understood from the diagrams and contour plots of visualized mechanical displacements obtained via the numerical procedure described in Ref. 16. All simulations were made with LT material constants reported in Ref. 12.

III. NUMERICAL RESULTS

A. Optimal cuts for wideband resonators with improved temperature performance

Maximum bandwidth of a resonator depends on the electromechanical coupling $k^2$ of the working mode and can be approximately estimated as $\Delta f_{r} = (f_A - f_R)/f_R$: hence, wideband resonators require high electromechanical coupling. Due to the lack of symmetry, none of the plate modes propagating in rotated YX-cuts can be referred to as pure SH or sagittally polarized (Lamb wave) modes. Therefore, the three zero-order modes described hereafter are distinguished as qSH0 (quasi-shear-horizontally polarized), qS0 (quasi-symmetric), and qA0 (quasi-anti-symmetric).

Similar to LN plates, in LT plates, the largest electromechanical coupling is assigned to qSH0 mode propagating in rotated YX-cuts. It is illustrated by Figure 2, which displays the characteristics of three zero-order modes as functions of rotation angle in rotated YX-cuts of LT. The normalized plate thickness $h_{LT}/2\rho$ varied between 0.1 and

![FIG. 2. Characteristics of zero-order modes propagating under an Al grating in rotated YX-plates of LiTaO3, with a plate thickness varying between $h_{LT}/2\rho = 0.1$ and 0.4, as functions of the rotation angle: (a) effective velocities of three modes at resonance ($V_{R1}$, $V_{R2}$, and $V_{R3}$); (b) electromechanical coupling; (c) temperature coefficients of frequency (TCF) of qSH0 mode estimated at resonance. Three BAW velocities in LiTaO3 (constant values $V_{p1}$, $V_{p2}$, and $V_{p3}$) are shown for reference. The contour plot in Figure 2(c) shows the structure of the qSH0 mode with displacement $u_0$ along the Y-axis.]}
0.4, while the aluminum electrode thickness was \( h_{AI}/2p = 0.01 \). The velocity of \( q_{A0} \) mode was most sensitive to variation of a plate thickness (Figure 2(a)). The coupling of \( q_{A0} \) and \( q_{S0} \) modes increased with a plate thickness but stayed low \( (k^2 < 3.5\%) \), while \( k^2 \) of \( q_{SH0} \) mode exhibited maximum value of 19.1% in 34° YX cut when \( h_{LT}/2p = 0.1 \) (Figure 2(b)). When \( h_{LT}/2p = 0.4 \), the coupling of \( q_{SH0} \) mode became twice smaller in the same orientation.

The TCF values were estimated at resonance for \( q_{SH0} \) as most attractive mode for wideband resonators. These values are shown in Figure 2(c) as well as the typical structure of \( q_{SH0} \) mode with dominant displacement \( u_2 \) parallel to the IDT electrodes and slowly decreasing with depth. TCF exhibited small positive values in the interval between 30° YX and 55° YX. This interval included three widely used in resonator SAW devices and therefore commercially available orientations: 36° YX, 42° LT, and 48° YX cuts. At anti-resonance, TCF was negative for any rotation angle with absolute value exceeding 30 ppm/°C.

For example, \( q_{SH0} \) mode propagating in 36° YX cut with the normalized plate thickness \( h/2p = 0.15 \) is characterized by \( V_R = 3845 \text{ m/s} \), TCF = -3.33 ppm/°C, and \( k^2 = 17.3\% \). These values are in a good agreement with the measured characteristics of the plate mode resonator reported in Ref. 4. The resonator was fabricated on 36° YX plate with thickness about 70 \( \mu \text{m} \) and \( \lambda = 2p = 430 \mu \text{m} \) and demonstrated resonance at \( f \approx 9.0 \text{ MHz} \) \( (V_R \approx 3870 \text{ m/s}) \) and TCF = -2.78 ppm/°C. The measured coupling \( k^2 = 13\% \) was lower compared to the value predicted theoretically because of the short length \( \lambda = 7\lambda \) of the IDT used for excitation and reflection of \( q_{SH0} \) mode.

Orientation 42° LT located in the middle of the angular interval of positive TCFs was further investigated as an example of the optimal cut for wideband plate mode resonators with improved temperature characteristics. Figure 3 shows the calculated velocities \( V_R \) of zero-order and higher-order plate modes propagating in this cut under an Al grating. The velocities of \( q_{SH0}, q_{S0}, \) and \( q_{A0} \) modes are displayed as functions of the normalized plate thickness \( h_{LT}/2p \). Multiple higher-order modes can be observed at \( h_{LT}/2p > 0.2 \). For reference, the velocities of three BAWs propagating along X-axis in LT \( (V_{B1-LT}, V_{B2-LT}, \) and \( V_{B3-LT}) \) and the velocity of the longitudinal BAW propagating in aluminum \( (V_{B1-AI}) \) are shown in the figure. It should be mentioned that in very thin LT plates \( q_{S0} \) mode can propagate faster than the longitudinal BAW because of accelerating effect of Al electrodes when a metal thickness is comparable with a plate thickness.

With further increase of an LT thickness, \( q_{A0} \) and \( q_{S0} \) modes gradually merge into SAW, while \( q_{SH0} \) mode transforms into leaky SAW, which propagates along the surface of a half-infinite LT substrate and leaks into the slow shear BAW.

Figure 4 shows an example of admittance as a function of the normalized frequency \( f'/2pf \) obtained for plate mode resonator built on a 42° YX cut with LT thickness \( h/2p = 0.2 \). Hereafter, the normalized admittances \( Y/Y_0 \) are presented, where \( Y_0 = 2\pi C_0 \) and \( C_0 \) is the static capacitance. The largest resonance at \( f' = 3874 \text{ m/s} \) with anti-resonance at \( f' = 4150 \text{ m/s} \) belonged to the \( q_{SH0} \) mode. Weak resonance at \( f' = 1653 \text{ m/s} \) belonged to the \( q_{A0} \) mode and stronger resonance at \( f' = 5541 \text{ m/s} \) was caused by the \( q_{S0} \) mode. One of the higher-order modes with mixed polarization could be seen at \( f' = 9103 \text{ m/s} \). The structures of the four modes are displayed in Figure 4 as the wave motions \( u_1 \) and \( u_2 \) in the XZ (sagittal) plane and the colored contour plots of \( u_2 \) along the Y-axis (SH-component). In the analyzed orientation, the modes \( q_{A0} \) and \( q_{SH0} \) exhibited typical structures for anti-symmetric and SH-type modes, while \( q_{S0} \) resembled a quasi-bulk wave with mostly longitudinal polarization and negligible variation of displacements along the plate thickness. Further analysis revealed that with increasing LT thickness, the displacements of the \( q_{SH0} \) mode remained focused under the grating and the wave gradually transformed into the SH-type SAW.

The effect of a thin metal electrode at the bottom of the LT plate on the \( q_{SH0} \) mode behavior in the 42° YX cut is illustrated in Figure 5. The dispersion curves and admittance functions shown in Figures 5(a) and 5(b) refer to the structures of Figures 1(a) and 1(b), respectively. The dispersion parameter

![FIG. 3. Velocities of quasi-symmetric (\( q_{S0} \)), quasi-anti-symmetric (\( q_{A0} \)), quasi-shear-horizontal (\( q_{SH0} \)) zero-order and higher-order modes propagating in a 42° YX-cut of LiTaO\(_3\) with an Al grating as functions of the LiTaO\(_3\) thickness. The thickness of the electrodes is \( h_{AI}/2p = 0.01 \). Three BAW velocities in LiTaO\(_3\) and longitudinal BAW velocity in Al (constant values \( V_{B1-LT}, V_{B2-LT}, V_{B3-LT}, \) and \( V_{B3-AI} \)) are shown for reference.](image3)

![FIG. 4. Normalized admittance of an Al grating on a 42° YX LT plate with thickness \( h/2p = 0.2 \). The displacements are schematically shown as the diagrams in the sagittal plane and contour plots in the shear horizontal direction calculated at the resonant frequencies of the four modes.](image4)
D = (βp − β0)/β0, where β0 = π/p and βp are the wave numbers unperturbed or perturbed by interaction of the mode with a periodic metal grating, is plotted as a function of the normalized frequency: (a) without an additional electrode; (b) with the Al electrode on the plate bottom. The coupling k2 of the qSH0 mode was determined by the difference (V R2 − V R1) in Figure 5(a) and by the difference (V A1 − V A2) in Figure 5(b).

The frequency shift between the OC and SC dispersion curves characterized the coupling k2 of the analyzed mode. It was much higher in a structure without metal at the bottom (Figure 5(a)). In such a structure, the resonance occurred at the lower edge of the SC stopband, 2pV R1 = V A1, and the anti-resonance appeared at the upper edge of the OC stopband, 2pV R2 = V A2. Due to the certain symmetry of the analyzed orientation, V R2 = V A1. As a result, the two stopbands were summed to yield a large difference between resonance and anti-resonance and hence high coupling k2 = 17.9%. With metallization at the plate bottom (Figure 5(b)), the anti-resonance occurred at the lower edge of the OC stopband, while V R2 = V A2, and the coupling decreased dramatically. The described behavior of qSH0 mode in 42° YX looks similar to that in 36° YX cut but the effect of a metal film on the coupling is stronger for 36° YX cut.

The amplitude and phase of the complex reflection coefficient κ could be estimated as

\[
\text{abs}(\kappa) = \frac{\pi(f_{R2} - f_{R1})}{f_0},
\]

where

\[
\Delta_{1,2} = 2\pi(f_{A1,2} - f_0)/f_0,
\]

\[
f_0 = (f_{R1} + f_{R2})/2,
\]

and \(\kappa^*\) means the complex-conjugate value. Calculations using Eqs. (3)–(6) yielded abs(κ) = 15%, arg(κ) = 0° for the data shown in Figure 5(a) and abs(κ) = 7%, arg(κ) = 0° for the data shown in Figure 5(b).

Inside the optimal interval between 30° YX and 55° YX cuts with positive TCFs at resonance (Figure 2), the behavior of zero-order plate modes with variation of a plate thickness looks similar but the coupling and TCFs change slowly with rotation angle. Figure 6 compares k2 and TCFs of qSH0 mode at the boundaries and in the middle of this interval, in 30° YX, 42° YX, and 55° YX cuts, and demonstrates that orientations 30° YX–42° YX cuts can ensure better performance if applied in wideband plate mode resonators. In these cuts, zero TCF at resonance can be combined with k2 = 18%–19% when hLT/2p = 0.1–0.13. Low coupling of spurious modes qS0 and qA0 may be considered as additional advantages in a resonator based on the qSH0 mode. High electromechanical coupling, low or zero TCF and low spurious modes combined with the commercial availability of the 36° YX and 42° YX cuts make them the best candidates for plate mode wideband resonators with improved temperature performance.

The main drawback of the qSH0 mode in the 30° YX–42° YX cuts that limits its application in high-frequency resonators is the low velocity: \(V \approx 3700–4100\) m/s. To improve this parameter, a search was performed among qS0 modes propagating in rotated YX-cuts of LT. Unlike the qSH0 mode, the mode qS0 showed larger coupling when a plate had metal at the bottom. In thin plates, the qS0 mode propagated with velocities close to V B3 = 5589 m/s. To combine high velocity with maximum coupling, a plate thickness of approximately hLT/2p = 0.5 is preferred. However, at this thickness, the first-order mode qSH1 interacted with zero-order mode qS0, thus building two coupled modes with mixed polarizations. Figure 7 shows the calculated characteristics of these two modes in rotated YX-cuts as functions of rotation angle. Typical structures of both modes

![Figure 5](image-url)

**FIG. 5.** Dispersion parameter D and normalized admittance for the qSH0 mode propagating under open-circuit (OC) or short-circuit (SC) gratings in a 42° YX-LT plate of thickness hLT/2p = 0.13, as functions of the normalized frequency: (a) without an additional electrode; (b) with the Al electrode on the plate bottom. The coupling k2 of the qSH0 mode was determined by the difference (V R2−V R1) in Figure 5(a) and by the difference (V A1−V A2) in Figure 5(b).

![Figure 6](image-url)

**FIG. 6.** Coupling and TCFs estimated at resonance and anti-resonance for qSH0 mode in three rotated YX cuts as functions of the LiTaO3 thickness.

[This article is copyrighted as indicated in the article. Reuse of AIP content is subject to the terms at: http://scitation.aip.org/termsconditions. Downloaded to | IP: 85.143.106.101 On: Tue, 25 Aug 2015 12:34:43]
are presented in Figure 7(a). Both modes were polarized in the plane of crystal symmetry YZ. The best combination of mode characteristics, with velocities $V_R = 5333 \text{ m/s}$, $V_A = 5530 \text{ m/s}$, coupling $k^2 = 8.5\%$, TCF $= -7/30 \text{ ppm/°C}$ at resonance/anti-resonance, was obtained for mode 1 in the $5°$ YX-cut with metal at the plate bottom. Despite the moderate coupling, this mode could find application in resonators due to relaxed requirements for the plate thickness, low TCF values and velocities that are approximately 1.5 times higher than typical SAW velocities in LT.

**B. Optimal cuts for Lamb wave resonators**

If the propagation direction in rotated Y-cuts of LT is normal to the X axis (rotated Y-cut, X + 90° propagation), only sagittally polarized plate modes (Lamb waves) S0 or A0 can be excited by IDTs. Any SH wave is piezoelectrically uncoupled in these orientations. Figure 8 shows the dispersion curves and admittance function for the plate mode $S_0$ propagating under an Al grating in a 50° Y, X + 90°-cut with plate thickness $h_{LT}/2p = 0.1$. In the analyzed orientations, the reflection coefficient was generally complex. Therefore, the admittance function was characterized by two resonances and two anti-resonances. The frequency intervals $(V_{R2} - V_{R1})$ and $(V_{A2} - V_{A1})$ determined the stopbands in SC and OC gratings, $\Delta_{SC}$ and $\Delta_{OC}$, respectively.

The variation of $S_0$ mode characteristics with cut angle in rotated Y, X + 90°-cuts is illustrated in Figure 9. This...
mode arose from the longitudinal BAW with velocity $V_{B3}$ dependent on rotation angle. With increasing LT thickness, the velocity of the $S_0$ mode went down. Its coupling depended on orientation and LT thickness. For example, in the $125^\circ Y$, $X+90^\circ$-cut, $k^2$ decreased from 11% at $h_{LT}/2p=0.1\%$ to 7% at $h_{LT}/2p=0.4$. When $h_{LT}/2p>0.4$, the analyzed plate mode had a structure close to that of the perfect symmetric Lamb wave, but in thin plates, the mode structure was strongly influenced by the longitudinal BAW, which was characterized by a Poynting vector parallel to the surface but wave vector tilted into the bulk. As a result, such a mode appeared more complicated than the perfect Lamb wave $S_0$. Examples of the mode structure obtained at $h_{LT}/2p=0.1$ and $h_{LT}/2p=0.4$ are shown in Figure 9(a).

The orientation $125^\circ Y$, $X+90^\circ$ exhibited an attractive combination of characteristics including high velocities of $V\approx 6000\text{ m/s}$, high coupling up to 11%, moderate TCF $\approx -35\text{ ppt/}^\circ\text{C}$ at resonance and the absence of SH-polarized spurious modes. Figure 10 shows the characteristics of $S_0$, $A_0$, and higher-order Lamb waves in this orientation as functions of the plate thickness varying between zero and $h_{LT}=2p$. In thick plates, $S_0$ and $A_0$ modes merged into a Rayleigh-type SAW. The structures of the $S_0$ and $A_0$ modes obtained at $h_{LT}/2p=0.5$ are displayed in Figure 10(a).

Examples of calculated admittance functions are shown in Figure 11. They belong to the $S_0$ mode propagating under the Al grating in the $125^\circ Y$, $X+90^\circ$-propagation. Additional resonance observed at $h_{LT}/2p=0.6p$ and $h_{LT}/2p=0.9p$ disappears at $h_{LT}/2p=0.8p$, when the complex reflection coefficient becomes real.

The orientation $125^\circ Y$, $X+90^\circ$ cut, $X+90^\circ$-propagation, as functions of the LiTaO$_3$ thickness: (a) effective velocities at resonance and wave structures calculated at $h_{LT}/2p=0.5$; (b) electromechanical coupling of the $S_0$ mode. In thick plates, $S_0$ and $A_0$ modes merged into a surface acoustic wave with velocity $V_{SAW}$. The orientation $125^\circ Y$, $X+90^\circ$ exhibited an attractive combination of characteristics including high velocities of $V\approx 6000\text{ m/s}$, high coupling up to 11%, moderate TCF $\approx -35\text{ ppt/}^\circ\text{C}$ at resonance and the absence of SH-polarized spurious modes. Figure 10 shows the characteristics of $S_0$, $A_0$, and higher-order Lamb waves in this orientation as functions of the plate thickness varying between zero and $h_{LT}=2p$. In thick plates, $S_0$ and $A_0$ finally merged into a Rayleigh-type SAW. The structures of the $S_0$ and $A_0$ modes obtained at $h_{LT}/2p=0.5$ are displayed in Figure 10(a).

Examples of calculated admittance functions are shown in Figure 11. They belong to the $S_0$ mode propagating under the Al grating in the $125^\circ Y$, $X+90^\circ$ plate with thicknesses of $0.6p$, $0.8p$, and $0.9p$. The phase $\arg(\kappa)$ of the complex

![Figure 10](image-url)

**FIG. 10.** Characteristics of $S_0$ and $A_0$ zero-order Lamb waves and higher-order plate modes in a $125^\circ Y$-cut, $X+90^\circ$-propagation, as functions of the LiTaO$_3$ thickness: (a) effective velocities at resonance and wave structures calculated at $h_{LT}/2p=0.5$; (b) electromechanical coupling of the $S_0$ mode. In thick plates, $S_0$ and $A_0$ modes merged into a surface acoustic wave with velocity $V_{SAW}$.

![Figure 11](image-url)

**FIG. 11.** Variation of the normalized admittance of the $S_0$ mode with plate thickness in a $125^\circ Y$-cut of LiTaO$_3$, $X+90^\circ$-propagation. Additional resonance observed at $h_{LT}=0.9p$ and $h_{LT}=0.9p$ disappears at $h_{LT}=0.8p$, when the complex reflection coefficient becomes real.

![Figure 12](image-url)

**FIG. 12.** Velocities and coupling of three first-order plate modes in rotated YX-cuts of LiTaO$_3$, $h_{LT}/2p=0.1$, as functions of rotation angle: (a) without additional electrode; (b) with Al electrode at the plate bottom. Typical structures of three modes are shown in Figure 12(a).

![Figure 13](image-url)

**FIG. 13.** Examples of simulated admittances for resonators using higher-order mode in $120^\circ YX$ plate with fixed thickness $h_{LT}=0.5\mu m$ and different periods of Al grating.
reflection coefficient $\kappa$ changed with LT thickness and crossed zero when $h_{LT} = 0.8p$. As a result, the second resonance coincided with the first anti-resonance and degenerated. These numerical examples demonstrate that the perfect admittance without spurious resonance can be obtained by tuning the plate thickness or geometrical parameters of the grating.

C. Optimal cuts for high-frequency resonators

Higher-order plate modes are extremely attractive for application in gigahertz resonators. The velocities and coupling of three first-order modes propagating in rotated YX-cuts with plate thickness $h_{LT}/2p = 0.1$ and Al film present or absent at a plate bottom are plotted in Figures 12(a) and 12(b) as functions of the rotation angle. The typical structures of the modes are displayed in Figure 12(a).

Mode 3 could be identified as qSH$_1$ with minor contribution of vertical displacement component. Modes 1 and 2 have mixed polarization and cannot be attributed to a certain type. Metallization of the plate bottom resulted in enhanced piezoelectric coupling of modes 2 and 3 but weakened coupling of mode 1. Figure 12 allows one to locate the optimal cuts based on the maximum coupling for each of the three modes: 110°–130° YX-cuts for mode 1 with velocities $V \approx 19,000$ m/s and maximum $k^2 = 14\%$, 150°–170° YX-cuts for mode 2 with velocities $V \approx 17,500$ m/s and $k^2$ up to 11%, and 0°–10° YX cuts for mode 3 with velocities $V \approx 18,000$ m/s and $k^2$ up to 10%. Metallization of a plate bottom was added to obtain the couplings mentioned above for modes 2 and 3. Very high velocities between 16,000 m/s and 20,000 m/s obtained at $h_{LT}/2p = 0.1$ decrease to $V = 10,000$–14,000 m/s when $h_{LT}/2p = 0.2$, as reported in Ref. 5, but the found intervals of rotation angles providing high coupling of each mode change insignificantly.

Minimum achievable plate thicknesses are usually limited by fabrication technologies, especially in high-frequency resonators. For LiNbO$_3$, minimum reported plate thickness used in experimental plate mode resonators was 0.5 $\mu$m.\(^{13}\) Figure 13 shows three examples of simulated admittance functions for resonators using LT plates with the fixed thickness $h_{LT} = 0.5 \mu$m. The periods of electrode structures were estimated to satisfy the normalized plate thicknesses $h/2p = 0.1$, 0.2, and 0.3. For each example, the main parameters of a resonator were estimated: resonant frequency $f_{0b}$, the relative bandwidth $\Delta f/f_{0b}$, and TCF at resonance.

The advanced numerical technique SDA-FEM-SDA was applied to investigation of plate modes propagating parallel or normal to X-axis in rotated Y-cuts of LiTaO$_3$ with periodic metal grating on top and metal film present or absent at a plate bottom. Effective velocities, electromechanical coupling coefficients, and temperature coefficients of frequency were calculated for zero-order and higher-order modes as functions of cut angle and plate thickness. Optimal cuts providing electromechanical coupling higher than 10% required for wideband resonators were found for qSH$_0$ and three first-order modes propagating in rotated YX cuts and for symmetric Lamb wave propagating in rotated Y-cuts, 90°-propagation. In thin plates with normalized thickness $h/2p = 0.1$, high coupling can be combined with low or zero TCF and velocities up to 20,000 m/s. The characteristics of zero- and first-order modes propagating in the determined intervals of optimal orientations are summarized in Table I.

![TABLE I. Plate mode characteristics in the optimal orientations of LiTaO$_3$.](image)

<table>
<thead>
<tr>
<th>Or ientations</th>
<th>$h_{LT}/2p$</th>
<th>Mode</th>
<th>$V$ (m/s)</th>
<th>$k^2$ (%)</th>
<th>TCF at resonance (ppm/°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30°–42° YX</td>
<td>0.1</td>
<td>qSH$_0$</td>
<td>3700–4200</td>
<td>18–19</td>
<td>0–5</td>
</tr>
<tr>
<td></td>
<td>0.2</td>
<td>qSH$_0$</td>
<td>3800–4200</td>
<td>15–16</td>
<td>(–10–12)</td>
</tr>
<tr>
<td>120°–130° YX</td>
<td>0.1</td>
<td>$S_0$</td>
<td>5800–6200</td>
<td>10–11</td>
<td>(–35–37)</td>
</tr>
<tr>
<td>110°–130° YX</td>
<td>0.1</td>
<td>Mixed</td>
<td>19,000–21,000</td>
<td>13–14</td>
<td>(–2–15)</td>
</tr>
<tr>
<td></td>
<td>0.2</td>
<td>Mixed</td>
<td>11,000–12,000</td>
<td>9–10</td>
<td>(–25–35)</td>
</tr>
<tr>
<td>155°–165° YX</td>
<td>0.1</td>
<td>Mixed</td>
<td>17,000–19,000</td>
<td>10–11</td>
<td>(–25–35)</td>
</tr>
<tr>
<td></td>
<td>0.2</td>
<td>Mixed</td>
<td>9000–10,000</td>
<td>8.5–10.5</td>
<td>(–23–32)</td>
</tr>
<tr>
<td>0°–10° YX</td>
<td>0.1</td>
<td>qSH$_1$</td>
<td>17,000–19,000</td>
<td>7.5–10</td>
<td>(–35–55)</td>
</tr>
<tr>
<td></td>
<td>0.5</td>
<td>qSH$_1$</td>
<td>5300–5500</td>
<td>8.1–8.5</td>
<td>(–7–9)</td>
</tr>
</tbody>
</table>

*aWith bottom electrode.*

\(^{1}\)J. Bjarstrom, I. Katardjiev, and V. Yanchev, Appl. Phys. Lett. 86, 154103 (2005).


