Correspondence

Theoretical and Experimental Study of Plate Acoustic Waves in ZX-Cut Lithium Niobate

Victor Klymko, Andriy Nadtochiy, and Igor Ostrovskii

Abstract—In this work, we report theoretical and experimental results on the 8 lowest modes of plate acoustic waves (PAW) propagating along the z-axis in the Z-cut of LiNbO$_3$ wafers (the “ZX-cut”). Dispersion curves are calculated by the method of partial waves and by the Finite Element Method (FEM); the curves are then measured experimentally. The spectra obtained by the 2 methods are in good agreement with each other and with the experimental results. The PAW modes are identified as components of the total acoustic displacements near cutoff frequencies. Electromechanical coupling efficiency of the 8 modes is described. The FEM work is verified by an application to the design and testing of a PAW delay line in a ZX-cut LiNbO$_3$ wafer. These results may be useful for analysis of many devices fabricated in Z-cut wafers, such as acousto-electric and acousto-optic components, ultrasonic motors and actuators, micro/nano-particle transporters, and other devices employing periodically poled ferroelectric waveguides.

I. INTRODUCTION

PLATE acoustic waves (PAW) in isotropic media were described in the mid-1960s [1], [2]. This work was extended to applications in a crystalline material, LiNbO$_3$ (LN), in the 1970s [3], [4]. Subsequently, the excitation of PAW in nonlinear acousto-electric and acousto-optic applications was reported in plates of CdS [5], LN [6]–[9], quartz [10], and KNbO$_3$ [11]. Basic properties of these waves, in particular the effects of dispersion [6], [12] and electromechanical coupling [12], [13], are topics for continued study. Theoretical analysis of PAW can be done employing the well-known method of partial waves [1]–[4] or the Finite Element Method (FEM) [14]. Thin plates of piezoelectric crystalline materials are extensively used as acoustic waveguides, in which the direction of wave propagation is orthogonal to the crystallographic cut of the material. However, the important Z-cut, with X-propagating PAW (ZX-cut), has not been considered in sufficient detail. Z-cut wafers of LN are extensively used in the design of periodically poled devices for laser harmonics generation and for other applications in acousto-optics [15], [16]. In addition, periodically poled ferroelectric vibrators operating at “domain resonance” [17] are designed using this ZX-cut. In the present work, we extend the understanding of the basic properties of PAW in ZX-cut LN, both theoretically and experimentally, and demonstrate some specific advantages of FEM. The FEM results compare favorably with those of the traditional method of partial waves, and are validated experimentally. Application to design of a PAW delay line is then described.

II. DISPERSION CURVES

The dispersion curves are first calculated by the well-known method of partial waves [1]–[4]. The equations of motion for a piezoelectric plate, along with the equations of electrodynamics and corresponding boundary conditions [3], [4], are solved for the crystallographic orientation under study. We use the elastic, piezoelectric, and dielectric constants, and material density from [18]. The dispersion curves computed by the partial wave method are presented in Fig. 1. The modes are enumerated from 1 to 8 in order of their occurrences as a function of an increasing dimensionless frequency $\Omega = (\omega b/\pi V_t)$, where $\omega$ is circular frequency, $b$ is the plate thickness, $V_t$ is the plate thickness, $V_t = (C_{44}/\rho)^{1/2}$ is the speed of the bulk shear acoustic wave propagating along the Z-axis. The horizontal axis is the dimensionless wave number $\beta b = (2\pi/\lambda) \times b$, where $\lambda$ is the ultrasound wavelength. The FEM model [14], [19], [20] allows solving the combined problem consisting of both propagation and excitation of PAW. We use the 2-dimensional FEM model, in which a plate is assumed to be infinite along the y-axis. A mesh consists of an arrangement of right triangular elements, each with sides of length $h_m$ in the x and z directions within the waveguide material (see the insert in Fig. 2). The mesh extends into the air as well. Computer simulation suggests that a boundary layer of air of thickness equal to $50 \times b$ is sufficient for an accurate solution; further increase in the air thickness does not change the spectrum of a PAW. Energy loss in a waveguide is represented by the imaginary part $c''$ of the elastic constants: $c_{ijkl} = c'_{ijkl} + ic''_{ijkl}$. We put $c''_{ijkl} = -0.002c'_{ijkl}$, which corresponds to a typical mechanical quality factor for a LN wafer of the order of 500. Absorbing loads at both ends of the plate (in the x-direction) are added to simulate an infinite-length-plate to eliminate the influence of reflections from the waveguide edges. The FEM simulation yields the acoustic amplitudes $U_{x,y,z}(\omega, x_i)$ for the set of frequencies $\omega_j$ at nodes $x_i$ on the plate surface along the direction of propagation. The discrete spatial Fourier transform is applied to obtain 3 components $U_{x,y,z}(\Omega_j, \beta_i)$ of the Fourier image of the displacements in the dimensionless frequency/wave-vector domain. The synthetic dispersion spectrum is visualized in a grayscale display of the total Fourier image given by.

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The authors are with the Department of Physics and Astronomy, University of Mississippi at Oxford (e-mail: iostrov@olemiss.edu).

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To limit the approximation error, it has been established \([20]\) that \(\lambda/h_m > 10\), where \(h_m\) is the side length of each mesh element inside the plate. In our numerical model, we use the plate thickness \(b = 0.5\) mm (because that is the thickness of the plate purchased for the experimental work) such that the above requirement is satisfied for \(\beta b < 6.28\). The synthetic dispersion spectra obtained by the FEm simulation are shown in Fig. 2, in which whiteness in the image is proportional to the magnitude of the Fourier images \(U(\Omega_j, \beta_i)\) of the corresponding PaW modes. The curves in Fig. 2 are numbered 1 through 8 to denote the corresponding PaW modes seen in Fig. 1. There is good agreement between the families of dispersion curves in Figs. 1 and 2, which establishes the validity of the FEm simulation compared with the well-known method of partial waves. It is important to note that the PaW spectrum of Fig. 2 remains the same if we plot any component of the displacement \(U_{x,y,z}(\Omega_j, \beta_i)\), or a sum of \(U_z(\Omega_j, \beta_i)\) plus the surface electric potential. However, for different displacement components there would be differences in the contrast between the gray background and the dispersion curves’ whiteness. To properly identify the PaW modes, one can analyze the acoustic displacements on the wafer surface for each mode near its cutoff frequency. This method is different from that used for isotropic plates in \([1]\) and \([2]\), where plate thickness is compared with the wavelength of the bulk acoustic wave at cutoff frequency. The mode identification obtained from the FEm simulation is given in Table I. These data are computed near cut-off frequencies at \(\beta = 0.1 \times 2\pi\) mm\(^{-1}\). Calculation by the traditional method of partial waves gives the same results, which strongly supports the FEm approach to computation of PaW modes.

In Table I, the maximum amplitude component along the \(x\)-, \(y\)-, or \(z\)-direction for a given mode is taken to be unity, such that other displacement components along the 2 remaining directions are fractions of the dominant component. Modes \(SS_0\), \(SA_1\), and \(SS_1\) are shear horizontal SH-type waves and other modes are Lamb-type PaW.

The dispersion curves were experimentally measured from 2 samples of single crystalline plates. The waveguide is an optical grade LN wafer, 0.5 mm thick and 76.2 mm in diameter, with both surfaces optically polished (MTI Corporation, Richmond, CA). The accuracy of crystallographic cut is <5′ for the \(z\)-axis, and <10″ for the \(x\)- and \(y\)-axes. Metal electrodes on the top and bottom surfaces

\[
U(\Omega_j, \beta_i) = \sqrt{[U_x(\Omega_j, \beta_i)]^2 + [U_y(\Omega_j, \beta_i)]^2 + [U_z(\Omega_j, \beta_i)]^2}. \tag{1}
\]

| Mode number | \(f\) (MHz) | \(\beta/2\pi\) (mm\(^{-1}\)) | \(u_x\) | \(u_y\) | \(u_z\) | Mode type |
|-------------|-------------|-----------------|--------|--------|--------|-----------|
| 1           | 0.08        | 0.1             | 0.146  | 0.001  | 1       | \(A_0\)   |
| 2           | 0.43        | 0.1             | 0.025  | 1       | 0.001  | \(SS_0\)  |
| 3           | 0.64        | 0.1             | 0.02   | 0.03  | 0.049  | \(S_0\)   |
| 4           | 3.60        | 0.1             | 0.023  | 1       | 0.003  | \(SA_1\)  |
| 5           | 4.23        | 0.1             | 0.01   | 0.03  | 0.101  | \(A_1\)   |
| 6           | 6.92        | 0.1             | 0.058  | 1       | 0.025  | \(SS_1\)  |
| 7           | 7.09        | 0.1             | 0.541  | 0.013  | 1       | \(S_2\)   |
| 8           | 7.44        | 0.1             | 0.001  | 1       | 0.001  | \(A_0\)   |

Fig. 1. Frequency spectrum of PaW in a ZX-cut LN wafer calculated by the partial wave method for \(b = 0.5\) mm. 1 – \(A_0\), 2 – \(S_0\), 3 – \(S_0\), 4 – \(SA_1\), 5 – \(A_1\), 6 – \(S_1\), 7 – \(SS_1\), 8 – \(S_2\). The insertion shows the orientation of the plate with respect to the direction of wave propagation.

Fig. 2. Frequency spectrum of PaW in a ZX-cut LN wafer calculated by the FEm simulation for \(b = 0.5\) mm. 1 – \(A_0\), 2 – \(S_0\), 3 – \(S_0\), 4 – \(SA_1\), 5 – \(A_1\), 6 – \(S_1\), 7 – \(SS_1\), 8 – \(S_2\). Insertion shows a fragment of the mesh used in the FEm model (not to scale).
of the samples were used to excite PAW, and special pickups were used to detect propagating modes, as shown in the insert of Fig. 3. We took the experimental data from a 40-mm-long central part of the wafer. We used a small ultrasonic transducer and a second metal electrode to read the acoustical displacement $U_z(t_n, x_m)$, and the electric potential $\phi(t_n, x_m)$, respectively, at a set of discrete points $x_m$ over the sample surface. The discrete readings of the pickup are taken at $N$ different times $t_n$ ($n = 1, 2, \ldots, N$) corresponding to each stop point $x_m$ ($m = 1, 2, \ldots, M$). Then, the discrete double Fourier transform is applied to the $N \times M$ matrix of the output data. The result of the double Fourier transform is the discrete function $U(\Omega_j, \beta_i)$ that represents either the acoustic displacement $U_1(\Omega_j, \beta_i)$ or the electric potential at the crystal surface, depending on the pickup used. For statistical reasons, we made multiple runs of the measurements from each sample, and the data were almost indistinguishable. The data shown are representative of those we acquired. In Fig. 3, a gray-scale plot of the functions $U(\Omega_j, \beta_i)$ shows a set of experimental synthetic dispersion curves in the frequency/wave-number domain. Fig. 3 is obtained as the sum of 2 sets of the data taken with the acoustical and electrical pickups, respectively, that is, $U_1(\Omega_j, \beta_i)$ plus surface electric potential. In addition to the propagating PAW modes denoted by the numbers 1 through 8 in Fig. 3, one can also notice a trace of a horizontal line near $\Omega = 1$. This is a reaction of the pick-up on the standing vibrations of the plate when its thickness is close to a half wavelength of a shear bulk wave propagating along the $z$-axis.

Analysis of Figs. 1–3 shows that the experimental data are in general agreement with both sets of calculations. However, in the experimental results some modes are not revealed at all frequencies. The modes 1, 2, 4, 5, and 8 are reliably detected in a relatively wide frequency range. Another 2 modes, 3 and 7, are observed in the more narrow frequency bands corresponding to $1.3 < \Omega < 1.6$ for zero symmetrical mode 3, $S_0$, and $2.2 < \Omega < 2.4$ for the first shear symmetrical mode 7, $SS_1$. Finally, the mode 6, $S_1$, shows up as a small white dash near its cutoff frequency $\Omega = 2$ near $\beta_0 = 0$. To understand the results of Fig. 3, and to identify possible acousto-electric applications, we have to know the electromechanical coupling or excitation efficiency [12], [13] ($K^2$) for the modes under consideration.

### III. Electromechanical Coupling

#### A. Method 1

$K^2$ may be calculated by 2 different approaches. For surface acoustic waves (SAW), the most frequently used method exploits the difference between the phase speeds $V_0$ and $V_M$ for surface waves in a piezoelectric waveguide with free and metalized surfaces, respectively [21], [22].

$$K^2 = [1 - (V_M / V_0)^2]$$ (2)

For small $K^2$, (2) may be simplified as $K^2 = 2(V_0 - V_M)/V_0 = 2\Delta V/V_0$.

In terms of the dimensionless frequency $\Omega$ and wave number ($\beta_0$), (2) becomes

$$K^2 = \left[1 - \left(\Omega M/(\beta_0) M\right)^2\right].$$ (3)

#### B. Method 2

The second approach is based on the effective permittivity $\varepsilon_S$, which in turn depends on acoustic wave slowness $s = \beta/\omega$, wave vector $\beta$, plate thickness $b$, and electrical characteristics of plate surface. This method was described in 1977 [23], and recently was shown to be appropriate for Lamb waves [24]. One can obtain a plot of $\varepsilon_S(s, \beta b)$ as a function of slowness $s$, and find slowness for the 2 cases of opened ($s_0$) and metalized ($s_M$) surfaces [23], [24]. The obtained $s_0$ and $s_M$ are further used to calculate $K^2$ by (2) using the equalities $V_0 = 1/s_0$ and $V_M = 1/s_M$. Some theoretical and experimental data for $K^2$ are shown in Fig. 4. We made calculations by both methods. For values of $K^2$ less than about 4 to 5%, which corresponded to modes 1, 3, 4, and 7, both approaches gave practically identical results. There is general agreement between previously published values of $K^2$ for zero-order modes [11] and the values shown in Fig. 4. In particular, the $K^2$ of mode 1, $A_{01}$, has a peak value of 1.8% in [11], and its maximum in Fig. 4 is 1.82%. The maximum $K^2$ of mode 2, $S_{02}$, is 14%, in [11] and the values calculated by simplified (2) and (3) are 14.1% and 13.6%, respectively. For mode 3, $S_0$, $K^2$ is zero for thin plates [11], and our value is less than 0.005% for $\Omega < 1$.

In Fig. 4, the $K^2$ plots for the dispersive modes 5, 6, and 8 are calculated by (3). They correlate well with the
intensity of experimental dispersion curves in Fig. 3. Mode 1, \( A_0 \), is observed to be well within the range \( 0.1 < \Omega < 1 \), and in the same range of frequencies the \( K^2 \) of this mode varies from 0.95% to its maximum value of 1.82%. Mode 2, \( S_{S_0} \), was observed in the experiment to be \( 0.01 < \Omega < 1.5 \), which corresponds to its \( K^2 \) plot in Fig. 4. Mode 3, the zero symmetrical mode \( S_0 \), is excited in the narrow range of \( \Omega \sim 1.5 \pm 0.1 \), and at these frequencies, its \( K^2 \) has a maximum of about 1%. Modes 4, \( S_{A_1} \), and 5, \( A_1 \), are detected at frequencies of \( 1.25 < \Omega < 2.3 \) for \( S_{A_1} \) and 1.1 \( < \Omega < 2.3 \) for \( A_1 \) (Fig. 3). These results are in agreement with the \( K^2 \) of modes 4 and 5 in Fig. 4. For mode 6, \( S_1 \), the short white dash in Fig. 3 at \( \Omega \sim 1.98 \), near \( \beta_b = 0 \), is the only part of the dispersion curve observed in the experiment. The \( K^2 \) for this mode has a narrow peak of \( \sim 4.5\% \) at this frequency. The shear horizontal mode 7, \( S_{S_1} \), is observed in Fig. 3 near \( \Omega = 2.35 \), which corresponds to its peak value of \( K^2 = 2\% \) at this frequency. The experimental dispersion curve of mode 8, \( S_2 \), is very intense at \( 2.1 < \Omega < 2.5 \), which is explained by its high \( K^2 \) of 10%–13.5% in this frequency range.

**IV. PAW DELAY LINE**

To verify the previous results we calculated and measured the transmission coefficient of a delay line based on a ZX-cut LN wafer. The input and output electrodes are 2-mm-wide metal strips on the top surfaces of the wafer. The length of the delay line is 30 mm. The result of the FEM computation is given in Fig. 5. It is important to note the FEM computation does not differentiate any PAW mode among those excited; it gives a total contribution of all excited PAW modes into delay line efficiency. In an experimental run, the same total contribution is detected. Experimentally, the transmission coefficient was measured with an Advantest 3131A network analyzer (Advantest Corporation, Tokyo, Japan); the results are presented in Fig. 6. There are 3 main bands observed in the theoretical and experimental data in Figs. 5 and 6. Their maxima are marked by numbers 5, 6 and 8, in accordance with the appropriate highest magnitudes of the piezoelectric coupling coefficients of corresponding PAW modes in Fig. 4. Since all excited modes with nonzero \( K^2 \) may contribute to delay line efficiency, the horizontal lines in Figs. 5 and 6 show the frequency ranges of these modes. For example, to the band at 3.6 to 4.3 MHz, besides mode 5, the modes 1, 2, and 4 may contribute. To the band at 7.2 to 7.9 MHz, 5 waves may contribute including modes 8, 7, 4, 2, and 1. The first band at \( 1.0 < \Omega < 1.2 \) corresponds to the maximum in \( K^2 \) of mode 5, \( A_1 \). The second narrow band marked 6 coincides with the maximum in \( K^2 \) of mode 6, \( S_1 \). Finally, the band at \( \Omega \) of \( \sim 2.1 \) to 2.3 is consistent with \( K^2 \) maximum of mode 8, \( S_2 \).

**V. CONCLUSIONS**

1) Dispersion curves for the first 8 PAW modes propagating along the \( x \)-axis in a Z-cut LN wafer can be calculated using the method of partial waves or the finite element method, both of which are in good agreement with each other and with experimental results. The FEM simulation has the particular advantage of providing information about the modeling of frequency sensitive devices using plate acoustic waves. However, a small discrepancy is observed at those frequencies and wave numbers, where more than one acoustic mode does exist. For instance, mode 7, \( S_{S_1} \), is expected to have its cutoff frequency
twice as high as mode 4, \( S_{A1} \), that is 7.2 MHz (\( \Omega = 2 \)), but the FEM simulation yields 7.09 MHz instead (1.5% inaccuracy).

2) The PAW modes can be identified by their \( x \)-, \( y \)-, and \( z \)-displacement components near the cutoff frequency of each mode. This method is particularly useful for identification of different PAW modes that may have the same cutoff frequencies, in which case the traditional method of counting the number of wavelengths along the plate thickness may lead to confusion.

3) Mode 8, the \( S_2 \) mode, appears to be the most promising choice for the design of a waveguide for transport of micro/nano-particles. This mode has respectively large amplitudes of both normal \( u_z \) and longitudinal \( u_x \) amplitudes near cutoff frequency and possesses relatively high electromechanical coupling efficiency of \( \sim 10\% \) at \( \Omega \sim 2.1 \) to 2.2. This can be seen from the amplitude components of PAW mode 8 in Table I, its coupling efficiency shown in Fig. 4, and the FEM simulation and experimental data of Figs. 5 and 6. The \( A_1 \) and \( S_2 \) modes are also indicated for use in other applications, such as delay lines.

4) The results described in this work may be useful for developing a wide range of acousto-optic and acousto-electric devices employing thin wafers of piezoelectric materials, such as surface acoustic wave devices, ultrasonic motors and actuators, or many other active acoustic devices that use thin plates of periodically poled crystalline materials.

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