Propagation Characteristics of Surface Acoustic Waves in AlN/128°Y-X LiNbO₃ Structures

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Abstract

In this study, propagation characteristics of surface acoustic waves (SAWs) in a layered piezoelectric structure consisting of an AlN thin film sputtered on 128°Y-X LiNbO₃ are investigated. The phase velocity and coupling coefficient of the layered structure with interdigital transducers (IDTs) and/or metal thin films deposited at various interfaces will be calculated numerically. The effects of the polarity of 128°Y-X LiNbO₃ on SAW characteristics are illustrated. By substituting the constituting relations into the Christoffel equations along with enforcing the appropriate boundary conditions on the interfaces, SAW characteristics of layered piezoelectric structures are determined by employing a matrix approach. Phase velocity and coupling coefficient of SAWs are presented versus h/λ, where h is the thickness of the AlN film and λ is the wavelength. Simulation results are compared with experimental data, which are calculated from S-parameter measurements of transversal SAW filters. A well matched comparison is demonstrated. Results obtained can be applied for the design of SAW devices using AlN/128°Y-X LiNbO₃ structures.

I. INTRODUCTION

128°Y-X LiNbO₃ substrate has been used extensively in the development of surface acoustic wave (SAW) devices, based on its excellent material properties such as a large piezoelectric coupling constant (5.36 %) and a high SAW velocity (3994 m/s). However, it has poor temperature stability (Temperature Coefficient of Delay, TCD = 75 ppm/°C).

The use of thin films to improve the temperature stability, phase velocity, or coupling coefficient of the substrate has been proposed and implemented by many researchers. Hickernell has addressed the role of thin-films played in SAW technology [1]. The zero temperature coefficient of frequency (TCF) structure using SiO₂/Y-Z LiTaO₃ has been reported by Parker and Wichansky [2]. The use of SiO₂ thin film sputtered on LiNbO₃ to achieve a high temperature stable SAW device with super high coupling has been reported by Yamanouchi and Ishii [3]. Kadota has widely investigated the effects of ZnO thin films sputtered on different substrates such as glass and quartz [4]. Nakamura and Hanaoka have studied the propagation characteristics of SAWs in ZnO/128°Y-X LiNbO₃ structures [5]. The mode coupling phenomenon between the Rayleigh and Love waves has been discussed and also the effects of the polarities between two piezoelectric media on characteristics of SAWs have been investigated. Characteristics of sputtering ZnO films on langasite and its SAW properties were reported by Wu et al. [6].

AlN and ZnO are the primary materials of piezoelectric films, and they have the same crystal structure, the hexagonal wurtzite structure. AlN thin films have some excellent characteristics, such as a high SAW velocity (nearly twice that of quartz and LiNbO₃), piezoelectricity, high-temperature stability, and stable chemical properties. Therefore, depositing AlN films on 128°Y LiNbO₃ may provide a new piezoelectric material for SAW devices. Characteristics of sputtering AlN films on 128°Y LiNbO₃ were examined [7] and their SAW properties were measured [8, 9]. Highly c-axis-oriented AlN films were achieved via the investigation of X-ray diffraction (XRD) [7]. Experimental results of transversal SAW filters revealed that 128°Y LiNbO₃ with an AlN film can increase the SAW velocity but at the expense of the decrease of coupling coefficient [9]. As h/λ increases, the absolute value of TCF decreases, which implies that the temperature stability of the substrate has been improved via an AlN film [9]. In order for using the proposed structure, AlN/128°Y-X LiNbO₃, to design SAW devices with the optimum performance, SAW characteristics have to be determined in the h/λ range of interest, which may be realized by employing a numerical approach. To the authors’ best knowledge, the corresponding numerical data have never been presented in the public domain.

To attain this goal, propagation characteristics of SAWs in AlN/128°Y-X LiNbO₃ are investigated in this study. Following the approach proposed by Campbell and Jones [10, 11], a matrix method is presented to determine SAW characteristics of layered piezoelectric structures with IDTs and/or metal thin films deposited at different
interfaces. Detailed derivations are discussed in Section II. Simulation results obtained versus h/2 are illustrated in Section III. The effects of the polarity of 128°Y LiNbO₃ on phase velocity and coupling coefficient will be elucidated. Simulated data are compared with measurement results, which are obtained from S-parameter measurements of transversal SAW filters [9]. A good agreement is presented. The last section is the conclusions.

II. METHOD OF ANALYSIS

The schematic of a layered piezoelectric structure, as depicted in Fig. 1, consists of an AlN film of thickness h and a 128°Y cut LiNbO₃ substrate. Note that the AlN film may be deposited on the positive surface or negative surface of the substrate. The angle between the positive surface normal and the Y-axis (crystallographic coordinate) is 128 degree, while for the negative surface is −52 degree. Highly c-axis-oriented AlN films were achieved on the substrate by rf magnetron sputtering, and are assumed to be independent of the substrate polarity [7]. Following the similar approach as developed by Campbell and Jones [10-12], a matrix method is employed here to calculate the SAW velocity in a layered piezoelectric structure.

![Fig. 1. Schematic of a layered piezoelectric structure consisting of an AlN film of thickness h and a 128°Y or −52°Y cut LiNbO₃ substrate. Rayleigh or leaky SAWs are assumed to be propagating along the x-axis.](image)

The acoustic and electric fields in media 1 and 2 can be expressed as

\[ u_j^{(1)} = \sum_{m=1}^{4} C_m a_j^{(m)} \exp(ikb^{(m)}z) \exp[i(kPx - \nu t)], \]

\[ j = 1, 2, 3, \]

\[ (1) \]

\[ \phi^{(1)} = \sum_{m=1}^{4} C_m \phi_j^{(m)} \exp(ikb^{(m)}z) \exp[i(kPx - \nu t)], \]

\[ (2) \]

\[ u_j^{(2)} = \sum_{m=1}^{8} C_m \alpha_j^{(m)} \exp(ikb^{(m)}z) \exp[i(kPx - \nu t)], \]

\[ (3) \]

\[ \phi^{(2)} = \sum_{m=1}^{8} C_m \alpha_j^{(m)} \exp(ikb^{(m)}z) \exp[i(kPx - \nu t)], \]

\[ (4) \]

where \( u \) is the acoustic displacement, \( \phi \) the electric potential, \( \nu \) the phase velocity, \( k \) the wave number in the x-direction, \( P = 1 + i\gamma \), \( \gamma \) is the attenuation coefficient, \( b \) and \( \beta \) the wave number ratios, and \( \alpha \) and \( \alpha \) the associated partial field amplitudes. Substituting eqs. (1) and (2) into stiffened Christoffel equations yields an eight-order algebraic equation in the wave number ratio \( b \). For each pair of values of \( (\nu, \gamma) \), there are eight real or complex values of \( b \). For a semi-infinite piezoelectric crystal, medium 1 in this case, four complex roots with negative imaginary parts are selected for a Rayleigh wave; meanwhile, in the case for a leaky SAW, one complex root, instead, has a positive imaginary part [13]. In the medium 2, eight roots of \( \beta \) are all selected.

The boundary conditions require that the acoustic displacements and stresses be continuous at \( z = 0 \) and the stress-free surface is assumed at \( z = h \). In addition, the electric potential and the normal component of electric displacement must be continuous at the interface for an electrically free surface. For a metallic (metal thin film) surface, the electric potential is vanished. Substituting eqs. (1)-(4) into boundary conditions, the phase velocity \( \nu \) and attenuation coefficient \( \gamma \) can be obtained numerically. The electromechanical coupling coefficient \( K^2 \) can be calculated from

\[ K^2 = \frac{2\nu_f - \nu_m}{\nu_f}, \]

where \( \nu_f \) and \( \nu_m \) are phase velocities obtained when the electrical boundary conditions at the interface at which the IDT is placed are assumed to be electrically free and shorted, respectively.

The phase velocities and coupling coefficients are calculated for the following four cases according to the positions of the IDT electrodes and/or metal thin films. (a) IDT/AlN/128°Y- or −52°Y-X LiNbO₃ (b) IDT/AlN/metal thin film/128°Y- or −52°Y-X LiNbO₃ (c) AlN/IDT/128°Y- or −52°Y-X LiNbO₃ (d) Metal thin film/AlN/IDT/128°Y- or −52°Y-X LiNbO₃. The matrix approach employed to compute the SAW propagation characteristics is detailed below. In the case (a), the IDT electrodes are placed on the \( z = h \) surface. At \( z = 0 \), by enforcing the boundary conditions, one can obtain

\[ M_{1u} \begin{bmatrix} C_m \end{bmatrix}_{4\times1} = \begin{bmatrix} M_{2u} \end{bmatrix}_{4\times8} \begin{bmatrix} X_m \end{bmatrix}_{8\times1}, \]

\[ (6) \]

while at \( z = h \) after simple manipulation yields

\[ M_{2u} \begin{bmatrix} X_m \end{bmatrix}_{8\times1} = 0, \]

\[ (7a) \]

for an electrically free surface and for an electrically shorted surface we obtain

\[ M_{2u} \begin{bmatrix} X_m \end{bmatrix}_{8\times1} = 0. \]

\[ (7b) \]

Substituting eq. (6) into eq. (7a) or eq. (7b) yields

\[ M_{1u} \begin{bmatrix} C_m \end{bmatrix}_{4\times1} = 0. \]

\[ (8) \]

The SAW phase velocities, \( \nu_{fa} \) and \( \nu_{ma} \) and the attenuation coefficients, \( \gamma_{fa} \) and \( \gamma_{ma} \), for the case (a) then can be determined by vanishing the determinant of the matrix \( M_{ua} \), i.e., \( det M_{ua} = 0 \), and, in turn, the acoustic and electric fields in media 1 and 2 can be obtained.

For the case (b), the IDT electrodes are still placed on the \( z = h \) surface, but a metal thin film is assumed to be deposited on the \( z = 0 \) plane. At \( z = 0 \), the electrical boundary conditions for cases (a) and (b) are significantly different from each other and, hence, eq. (6) is now modified to three sets of equations as given by

\[ M'_{1u} \begin{bmatrix} C_m \end{bmatrix}_{4\times1} = \begin{bmatrix} M'_{2u} \end{bmatrix}_{4\times8} \begin{bmatrix} X_m \end{bmatrix}_{8\times1}, \]

\[ (9a) \]
and from eq. (9b), one can obtain
\[ C_4 = C'_4 (C_1, C_2, C_3), \]
and also from eq. (9c) and one equation in eq. (7a) or eq. (7b) we can express \( X_1 \) and \( X_6 \) in terms of the rest \( X_{m,s} \) as given by
\[ X_1 = X_1 (X_2, X_3, X_4, X_5, X_6, X_7) \]
\[ X_6 = X_6 (X_2, X_3, X_4, X_5, X_6, X_7). \]
Substituting eqs. (10a)-(10c) into eq. (9a), and then using the rest equations in eq. (7a) or eq. (7b) yields
\[ [M_{1b}]^{x=1}[M_{mb}]^{x=1} = 0. \]

The measured effective velocity should be less than \( v_f \). For the IDT with metallization ratio 0.5, the effective velocity can be calculated from \( v_f \) and \( v_m \) as given by
\[ v_{eff} = \frac{v_f v_m}{v_f + v_m}. \]

### III. RESULTS AND DISCUSSION

The material constants of AlN and LiNbO₃ employed here were obtained from the study reported by Gualtieri et al. The phase velocities, for the case (a), presented in Fig. 2 are obtained by vanishing the determinant of the matrix \( M_{mb} \), as indicated in eq. (8). The subscripts 1 and 2 in \( v_{fa1} \) and \( v_{fa2} \) indicate the AlN film is deposited on the positive surface and negative surface of the substrate (denoted respectively by 128°Y and −52°Y cut LiNbO₃), respectively. Both \( v_f \) and \( v_m \) increase with increasing \( h/\lambda \), where \( h \) is the thickness of the AlN film and \( \lambda \) is the wavelength. This is because the Rayleigh wave velocity for AlN, around 5400 m/s, is greater than that for 128°Y-X LiNbO₃, 3994 m/s. When \( h/\lambda \) is around 0.013, the phase velocities, \( v_{fa1} \) and \( v_{fa2} \), approach 4079 m/s, which is the shear bulk wave velocity for 128°Y cut LiNbO₃. Therefore, a leaky wave solution to the substrate is searched when the SAW phase velocity is greater than 4079 m/s. The associated attenuation coefficients are presented in Fig. 3. The attenuation coefficient is zero for the Rayleigh wave and has a significantly large value for the leaky wave especially in the region when the SAW velocity is slightly higher than the shear velocity. Therefore, our discussion is mostly restricted on the Rayleigh wave region.

The value marked with a dot in Fig. 2 represents the measured effective velocity of transversal SAW filters. The measured velocity was obtained using \( v_{eff} = f_{00}^0 \lambda_0 \), where \( f_0 \) is the center frequency estimated in \( S_2 \), and \( \lambda_0 \) is the period of IDT. It is clear that the measured velocity has the same trend as the simulated data, i.e., the velocity increases as \( h/\lambda \) increases. The measured center frequency is shifted downward due to the effect of the slow phase velocity in the metallization region and, hence, the
\( K^2 \) denote the AlN film is deposited on the positive surface and negative surface of the substrate, respectively. This indicates that the polarity of the substrate may affect the SAW propagation characteristics. In the case (b), a metal thin film is deposited on the interface plane between AlN and LiNbO\(_3\) and, hence, the electric fields in AlN and LiNbO\(_3\) are isolated from each other; this causes the effects of polarity vanished and such that \( K^2_1 = K^2_2 \).

In Fig. 4(a), \( K^2_1 \) is greater than \( K^2_2 \) in the whole \( h/\lambda \) ranges of interest. In the Rayleigh wave region, say \( h/\lambda \) less than 0.013, \( K^2_1 \) increases from 5.36\% to a peak value of 5.58\%, at \( h/\lambda = 0.007 \) and then becomes decreasing. In the same region, \( K^2_2 \) decreases monotonically. Though a maximum value around 6.76\% is shown in \( K^2_1 \), it is occurred in the leaky wave region with the attenuation coefficient of a very large value, 2.51\( \times 10^{-3} \). The dot value in Fig. 4(a) is measured from \( S_{11} \) of transversal SAW filters [9]. The value of \( K^2 \) is calculated using [6, 9]

\[
K^2 = \frac{\pi}{4N} \frac{G_0}{B_0} \left| \frac{\eta}{\eta_0} \right| , \quad (13)
\]

where \( N \) is the number of IDT finger pairs, and \( G_0 \) and \( B_0 \) are radiation conductance and susceptance, respectively. It is obvious in Fig. 4(a) that the measured \( K^2 \) not only has the same trend as \( K^2_2 \) but its value is approximates that of \( K^2_2 \). This implies that the substrate for fabricating SAW devices is \(-52^\circ Y\) cut LiNbO\(_3\).

In Fig. 4(b), \( K^2_1 (= K^2_2) \) has a very small value as compared with the rest three cases. This illustrates that the metal thin film deposited on the interface plane between two piezoelectric media decreases the coupling coefficient significantly. For the case (c), \( K^2_1 \) and \( K^2_2 \) in Fig. 4(c) have almost the same values in the Rayleigh wave region. A peak value of 6.1\% is observed at \( h/\lambda = 0.01 \). Comparing Fig. 4(c) with Fig. 4(a), a peak value of 6.1 \% can be found in the Rayleigh wave region for the case (c) regardless of the polarity of the substrate. However, for the case (a) a peak is observed only in \( K^2_1 \).

The coupling coefficient with a metal thin film deposited on the top surface is presented in Fig. 4(d). The value of \( K^2 \) is smaller than that in Fig. 4(a) or Fig. 4(c) in the Rayleigh wave region. This shows that a metal thin film on the top surface may also decrease the coupling coefficient.

According to the simulation and measurement data presented in Figs. 4(a)-4(d), in the Rayleigh wave region the AlN/IDT/128°Y-X LiNbO\(_3\) structure can exhibit the best performance with a proper \( h/\lambda \) among all the cases investigated in this study, and, especially, the effects of the polarity of the substrate are almost vanished in the corresponding structure. This information can be employed as a design rule for the fabrication of SAW devices using AlN/128°Y-X LiNbO\(_3\) structures.
In this paper, a matrix method was employed to calculate the SAW phase velocity in a layered piezoelectric structure consisting of an AlN thin film sputtered on 128°Y-X LiNbO$_3$. Propagation characteristics of SAWs in different layered structures such as IDT/AlN/128°Y-X LiNbO$_3$ or metal thin film/AlN/IDT/128°Y-X LiNbO$_3$ with positive and negative polarities of the substrate were investigated and demonstrated versus various $h/\lambda$. For the IDT/AlN/128°Y-X LiNbO$_3$ structure, the effects of the polarity were apparent in the coupling coefficient; the calculated phase velocity and coupling coefficient were compared with experimental data. A well matched comparison is shown between the calculated and measured effective velocities. The measured coupling coefficient approximates the calculated data obtained with a negative polarity of the substrate, −52°Y cut LiNbO$_3$. In the Rayleigh wave region, the AlN/IDT/128°Y cut LiNbO$_3$ structure shows that the effects of the polarity of the substrate can be neglected and exhibits a highest coupling coefficient among all the cases studied in this paper. This information can be employed as a design rule for the fabrication of SAW devices using AlN/128°Y-X LiNbO$_3$ structures. Simulation results also indicate that a metal thin film deposited on the interface plane between two piezoelectric media can significantly decrease the coupling coefficient and in the Rayleigh wave region the metal thin film on the top surface will also decrease the coupling coefficient.

IV. Conclusions

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