Twist Piezoelectric Coupling Properties to Suppress Spurious Modes for Lithium Niobate Thin-film Acoustic Devices

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Abstract—This paper presents a new method to suppress spurious modes in lithium niobate thin-film acoustic devices by twisting the piezoelectric coupling properties of the spurious modes. The excellent piezoelectric properties of lithium niobate (LiNbO₃) advance performance but lead to significant spurious modes accompanied by the targeted main mode. To harvest the benefits and avoid the spurious modes, this work investigates solidly mounted LiNbO₃ thin films with different substrates to twist the zero-coupling orientations of spurious modes to be close to the maximum-coupling orientation of the targeted main mode. The fabricated devices, based on the solidly mounted LiNbO₃/sapphire structure and surface guided acoustic wave, show an operating frequency of 2.4 GHz with a large electromechanical coupling of 22% and a spurious-free response in the wide frequency range. This work could overcome a significant bottleneck in commercializing LiNbO₃ thin-film acoustic devices.

Keywords—Acoustic resonator, lithium niobate, sapphire, solidly mounted thin films, spurious mode suppression.

I. INTRODUCTION

To overcome the high loss in the traditional surface acoustic wave (SAW) devices for higher frequency 5G wireless communication systems, acoustic devices based on high-quality piezoelectric thin films (including aluminium nitride, lithium tantalite, and lithium niobate) are widely investigated from several GHz to mmWave [1]–[7]. Due to the recent development of single-crystal thin-film transfer and heterogeneous integration techniques, lithium niobate (LiNbO₃) thin films have shown promising potentials for ultra-wideband applications in 5G frequency bands. Various platforms for LiNbO₃ thin films, including suspended and solidly mounted structures, contribute to the vast room for innovative acoustic resonators/filters and different usage scenarios[8], [9]. To handle higher power in the radio frequency (RF) front ends, the solidly mounted structures for LiNbO₃ thin films, featuring efficient heat dissipation capability, have been demonstrated with large quality factors (Qs) and electromechanical couplings (K²) [9]–[11].

However, the excellent piezoelectric property of LiNbO₃ is a double-edged sword that the spurious modes accompany the main acoustic wave mode leading to interference with the front-end communication channels and signal distortion. The origins of the spurious acoustic modes in LiNbO₃ thin films can be categorized into two main types: direct and indirect excitations from the piezoelectric coupling [12]. The direct excitations of spurious acoustic modes are determined by the piezoelectric coupling properties of the material, while the indirect excitations are due to the mode conversions and reflections at various acoustic boundaries (e.g., transverse spurious modes and higher-order lateral spurious modes). For indirect excitations, several solutions based on different topologies of interdigital electrodes (e.g., rhombic weighted electrodes, oblique electrodes, and hammerhead electrodes) and reflectors have been widely investigated [13]–[15]. For direct excitation, as they are the intrinsic modes of the LiNbO₃, these spurious modes cannot be suppressed by adjusting the topologies and acoustic boundary conditions of transducers. The previous methods, which tuned the wavelength and metal ratios, focused on shifting these spurious modes out of the passband, leading to the limited range of operating frequencies [9], [10].

Considering LiNbO₃ is highly anisotropic, these intrinsic spurious modes feature various K² in different orientations, and zero-coupling points exist. This work proposes to twist the piezoelectric coupling properties of the spurious modes to be 0 at the orientations where the targeted main mode features large K². This work focuses on the solidly mounted LiNbO₃ thin films with different carrier substrates and utilizes the fundamental shear horizontal mode (SH0) as the main mode. To validate our analysis and modelling, resonators operating at 2.4 GHz are fabricated and demonstrated with a spurious-free response without sacrificing the K² of the main mode.

II. SURFACE GUIDED ACOUSTIC WAVES

A. Solidly Mounted Lithium Niobate Thin Film

Considering the limitation in K², the energy confinement has been conceived as the first key point to boost the coupling coefficients of targeted modes in LiNbO₃ thin films. Therefore, the design of LiNbO₃-based resonators should start from the selection of device configurations for confining acoustic waves in the piezoelectric material efficiently. Fig. 1(a) and (b) present the cross-section views of the suspended type and the solidly mounted type of acoustic wave resonators. Given energy confinement, the suspended structure features more distinct energy confinement by resorting to the maximum acoustic impedance mismatch between the air gap and LiNbO₃. However, resonators based on free-standing LiNbO₃ thin films usually exhibit poor power handling capability due to heat dissipation challenges. Enabled by better thermal conductivity and larger contact area, the solidly mounted type shows promising potential in advancing power handling performance [9], [10], [16]. Besides, acoustic waves can be well confined in the structure by engineering the acoustic velocity difference between LiNbO₃ and substrates.

In the thin-film LiNbO₃ solidly mounted structure, SH0 mode has been demonstrated with promising performance [9]–[11]. However, the fundamental asymmetric Lamb wave (A0)
features an acoustic velocity close to SH0 mode and significant $K^2$ at the optimized orientation for SH0 mode. As above mentioned, A0 mode is defined as the intrinsic spurious mode in the devices designed for SH0 mode. This work focuses on twisting the piezoelectric coupling properties of A0 mode to be 0 at the orientations where SH0 mode features large $K^2$.

To understand the A0 mode and the targeted SH0 mode, a 2.5D finite element analysis of the structures mentioned above is performed in COMSOL Multiphysics. Displacement mode shapes of these two modes are shown in Fig. 1(a) and (b), respectively. Based on the zoomed-in displacement distribution, the SH0 mode is well confined to the piezoelectric layer of the solidly mounted structure, while the displacement of A0 mode is affected by the carrier substrate. The new idea comes that the properties of A0 mode can be twisted by engineering the substrate.

**B. Twisting Piezoelectric Coupling Properties**

Due to the anisotropic essence of LiNbO$_3$, the piezoelectric coupling of SH0 mode and A0 mode vary from different propagation directions. Given this property, eigenmode analysis for LiNbO$_3$ thin film with different topologies and substrates is investigated for understanding how to twist the zero-coupling orientations of A0 mode to be close to the maximum coupling orientation of the targeted SH0 mode. Considering the wave dispersion of the targeted SH0 mode and in-house micro-fabrication capabilities for this work, the lateral wavelength of the SH0 mode (A0 mode) is set to be 1.6 µm for operating at 2.4 GHz. Due to the in-plane 180º symmetry, the material matrices of LiNbO$_3$ are rotated 180º around +Y axis using the Euler angle-based method for comparing $K^2$. $K^2$ of SH0 mode and A0 mode versus the rotation angles of LiNbO$_3$ in suspended and solidly mounted platforms are presented in Fig. 2-5, respectively. By comparing $K^2$ under different propagation directions, $\alpha$ is defined as the maximum-coupling orientation for the SH0 mode and $\beta$ is defined as the zero-coupling orientation for the A0 mode.

Fig. 2(a) shows the $K^2$ of A0 and SH0 mode as a function of device orientations in the suspended LiNbO$_3$ thin film. The coupling of both modes changes when the orientation varies from -90º to 90º along the +Y axis in the X-cut plane. As seen in Fig. 2(b), with the propagation direction along the -10º to +Y axis, SH0 mode features the highest $K^2$ of 36.49% and the coupling of A0 mode is 3.48%, which might lead to large ripples around the passband. As presented in Fig. 2(c), when the wave propagation direction is between 48º and 51º to +Y axis, the A0 mode features zero coupling and the $K^2$ of SH0 mode is below 5%. As the difference between $\alpha$ and $\beta$ is over 59º, it is hard to trade off between a large coupling of SH0 mode and a zero-coupling of A0 mode.

To narrow the gap between $\alpha$ and $\beta$, the further concern to us is to utilize the solidly mounted structure for twisting the properties of A0 mode. For solidly mounted structures, the carrier materials for LiNbO$_3$ thin films play a fundamental role in the generation and confinement of acoustic waves, as well as the achievable $K^2$, feasibilities, and costs. Amorphous silicon (a-Si), silicon oxide (SiO$_2$) and sapphire are evaluated to twist the $K^2$ of SH0 mode and A0 mode with respect to the in-plane orientations. Additionally, single crystal silicon (c-Si) is defined as the supporting substrate underneath a-Si and SiO$_2$ for integration consideration. As seen in Fig. 3, the LiNbO$_3$ on a-Si/c-Si platform delivers the highest $K^2$ (26.04%) of SH0 mode and the coupling of 1.92% for A0 mode at $\alpha$ (-8º). By rotating the propagation direction to $\beta$ (62º-67º), the A0 mode can be fully suppressed but the SH0 mode features a relatively...
low $K^2$ (< 2.5%). Similarly in the platform on SiO$_2$/c-Si (Fig. 4), both SH0 and A0 modes feature the maximized $K^2$ at the propagation direction of -9º to +Y axis, and the minimum difference between $\alpha$ and $\beta$ is 64º. Therefore, it is still challenging to achieve SH0 mode with a large $K^2$ (>10%) and suppressed A0 mode simultaneously. It is worth noting that the addition of a-Si and SiO$_2$ appears to have degraded the piezoelectrical coupling of acoustic waves compared to that of the suspended structure, which can be ascribed to the worse electrical field distribution in the thickness direction.

It is clear that the piezoelectric coupling properties of the SH0 and A0 modes are twisted in the previous two solidly mounted platforms but in the opposite direction to the purpose. This work found that sapphire can help to minimize the gap between $\alpha$ and $\beta$. Fig. 5 exhibits the simulated result under different orientations based on the LiNbO$_3$/sapphire platform. Unlike previous structures, a minimum difference of 22º between $\alpha$ and $\beta$ is achieved and it can be further minimized in the devices with top electrodes. Therefore, only extracted $K^2$ versus the in-plane orientation with a step of 1º based on the LiNbO$_3$/Sapphire structure.

C. Acoustic Spurious Mode Suppression

As the deposition of electrodes will adjust the stress field inside the LiNbO$_3$, the previously simulated $K^2$ based on the eigenmode analysis lays the ceiling before considering the mass and electrical loading effects brought by electrodes. Besides, the twisting angles will slightly shift from those of eigenmode analysis, and this is due to the change of equivalent material matrices and device topology after the addition of electrodes. Moving forward, frequency-domain simulations are utilized to validate the analysis of $\alpha$ and $\beta$ discussed above by considering the influences from top electrodes. The design parameters of acoustic wave resonators based on the above-mentioned four structures are listed in Table 1. As seen in the red curves of Fig. 6 (a)-(d), the devices designed in these structures to maximize the $K^2$ of SH0 mode can also excite significant A0 modes in the targeted frequency range. Consistent with the analysis, the coupling of SH0 mode is notably degraded at the orientation for fully suppressing A0 mode in the first three discussed structures [Fig. 6 (a)-(c)]. By slightly adjusting the orientation of transducers from -11º to 4º, the simulated responses of LiNbO$_3$/sapphire platform show that the in-band spurious mode can be fully suppressed without sacrificing the coupling of SH0 mode (Fig. 6(d)).
Fig. 7. Microscope image of the as-fabricated LiNbO$_3$/sapphire resonator.

Fig. 8. Measured admittance response of SH0 mode resonators based on the LiNbO$_3$/a-Si/c-Si and LiNbO$_3$/sapphire resonators.

III. IMPLEMENTATION AND MEASUREMENTS

To validate the analytical and modeling results, the devices were in-house fabricated on LiNbO$_3$ thin films, bonded on a c-axis sapphire wafer and 400 nm thick amorphous silicon on the (111) plane of a single-crystal silicon wafer, respectively. The microscope image of the fabricated resonator is shown in Fig. 7 with the zoomed-in view of the interdigital electrodes. The fabricated resonators were characterized at room temperature with a Keysight P5028A network analyzer and the responses are presented in Fig. 8. The experimental result based on LiNbO$_3$/a-Si/c-Si displays an SH0 mode at 2.52 GHz and a strong spurious mode (A0 mode) at 2.25 GHz. As a comparison, the device based on LiNbO$_3$/sapphire shows a spurious-free response with an effective electromechanical coupling ($k^2$) of 22%, which is even larger than the device with spurious coupling. Such results validate our proposed strategy for spurious-free LiNbO$_3$ thin-film acoustic devices.

IV. CONCLUSION

This work presents a new idea to suppress the intrinsically excited spurious mode based on the solidly mounted resonators by twisting the piezoelectric coupling properties of the spurious mode to be 0. The resonance behaviours of suspended and solidly mounted structures based on different carrier substrates are first investigated. The LiNbO$_3$/sapphire stands out among these structures since it can twist the zero-coupling orientations of the A0 to be close to the maximum-coupling orientation of the targeted SH0 mode. This work could contribute to the commercialization of LiNbO$_3$ thin-film devices. The proposed idea can be further applied to other targeted acoustic waves and structures/materials.

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