



## Article

# High-Frequency and Spectrum-Clean Shear-Horizontal Acoustic Wave Resonators with AlN Overlay

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**Abstract:** By bonding the sub-wavelength-thick lithium niobate ( $\text{LiNbO}_3$ ) layer to high-phase-velocity ( $v_p$ ) substrates, such as Si, the shear-horizontal (SH) modes no longer couple with the bulk modes leaking into substrates. As the propagation loss is no longer the major concern for these types of nonleaky SH wave devices, the YX- $\text{LiNbO}_3$  with a low rotation angle providing ultra-large coupling coefficient ( $k_{\text{eff}}^2$ ) can be used. In addition, by overlaying a high-velocity layer such as AlN on top of  $\text{LiNbO}_3/\text{Si}$ , the  $v_p$  of the SH wave can be significantly enhanced at a small cost of  $k_{\text{eff}}^2$ . By a careful design of the stack, both the wide-band spurious (Lamb wave) and near-band spurious (Rayleigh wave) are suppressed successfully. This paper focuses on the design of layered substrate not only to optimize its resonance characteristics—series frequency ( $f_s$ ), quality factor ( $Q$ ),  $k_{\text{eff}}^2$ , and temperature coefficient of frequency (TCF)—but also for eliminating the out-of-band spurious responses. The optimized substrate design demonstrates the minimal propagation loss, high  $f_s$  of 3 GHz, large  $k_{\text{eff}}^2$  of 14.4% and a spurious-free response at 0–6 GHz. These novel nonleaky SH wave devices can potentially enable the low loss and wideband processing functions, which is promising for the 5G/6G radio frequency (RF) communication systems.



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**Keywords:** aluminum nitride;  $\text{LiNbO}_3$ ; 6G; shear-horizontal mode; coupling coefficient

## 1. Introduction

The propagation-loss mechanisms of shear-horizontal (SH)-type waves on  $\text{LiNbO}_3$  and  $\text{LiTaO}_3$  have been intensively studied recently [1–6]. By bonding the sub-wavelength-thick  $\text{LiNbO}_3$  or  $\text{LiTaO}_3$  layer to a high-velocity substrate, the SH mode no longer couples with the bulk mode in substrate and the leaky component is effectively eliminated [1–6]; thus, the SH wave can abandon its traditional name—“leaky-surface acoustic wave (SAW)” but a favorable “nonleaky” feature instead. There are many choices of high-velocity substrates, such as AlN, Si, quartz, diamond, etc. [1–5], and Si is used as an example in this study for its wide availability and cheap price. In addition, given that the acoustic propagation loss no longer dictates the choice of piezoelectric-substrate cut angle and ultra-large effective coupling coefficient ( $k_{\text{eff}}^2$ ), cuts can be taken advantage of, such as low rotation from YX- $\text{LiNbO}_3$  [3–7].

Long-Term Evolution (LTE)—Advancement Pro, 5G sub-6 GHz new radio (NR), and emerging 6G standards require low-loss and wide-bandwidth (fractional bandwidth > 5%) filters that push the frequency limits SAW technology using optical lithography up to more than 2.5 GHz range [8–14]. That shrinking SAW resonators size enables the high frequency, while the quality-factor ( $Q$ ) significantly deteriorates. With the  $k_{\text{eff}}^2$  less than 10% and phase velocity ( $v_p$ ) less than 4500 m/s, the current commercially popular standard-SAW and Temperature Compensated Surface Acoustic Wave (TCSAW) devices can hardly meet the requirements. Intriguingly, the low-angle-rotated YX- $\text{LiNbO}_3$  provides ultralarge intrinsic  $k_{\text{eff}}^2$  (~30%). After  $\text{LiNbO}_3$  bonded to Si, the propagation-loss problem is resolved and

high  $Q$  is achieved [4]. The multilayered LiNbO<sub>3</sub> SAW devices with ultralarge  $k_{\text{eff}}^2$  and high  $Q$  meet requirements in low frequency (<2.5 GHz). However, the  $v_p$  is still relatively low (~4000 m/s), limiting its application in LTE high-band (2.5–3.5 GHz, such as band 7, band41, etc.) filters and 5G NR applications. A high-velocity layer beneath the piezoelectric LiNbO<sub>3</sub> or LiTaO<sub>3</sub> does not effectively increase the phase velocity of the SH mode; rather, by adding a high-velocity layer, such as AlN, overlaid on top of the transducer and LiNbO<sub>3</sub>, the phase velocity of the SH mode is visibly increased with only minimal trade-off on the  $k_{\text{eff}}^2$ , which can be much larger than needed for majority of the bands. In this way, a desirable nonleaky SH wave resonator with low propagation loss, high frequency ( $f$ ), and large- $k_{\text{eff}}^2$  can be achieved.

In addition, without a careful design of the substrate, the layered SH potentially has spurious responses in the out-of-band frequencies (Lamb modes) and near-band frequencies. This paper focuses on the design of layered substrate not only to optimize its narrow-band characteristics— $f$ ,  $Q$ ,  $k_{\text{eff}}^2$ , temperature coefficient of frequency (TCF)—but also for eliminating the out-of-band spurious responses.

By using the numerical calculation and finite-element-method (FEM) approaches, propagation characteristics of the SH modes in LiNbO<sub>3</sub>/Si and AlN/LiNbO<sub>3</sub>/Si are derived with varied substrate designs and the device performance is optimized as well as the presence of spurious modes avoided. Based on the analyses, new stacks with optimized substrate design are obtained, demonstrating the high frequency of 3 GHz at 1  $\mu\text{m}$  interdigital transducer (IDT) pitch, high  $k_{\text{eff}}^2$  (14.4%) and a spurious free response at 0–6 GHz. After optimizations, these novel AlN/LiNbO<sub>3</sub>/Si nonleaky SH devices, featuring superb performance with high frequency ability and being spurious-free, show great potential for filters in next-generation RF front ends.

Symbols used in this paper are listed in Table 1.

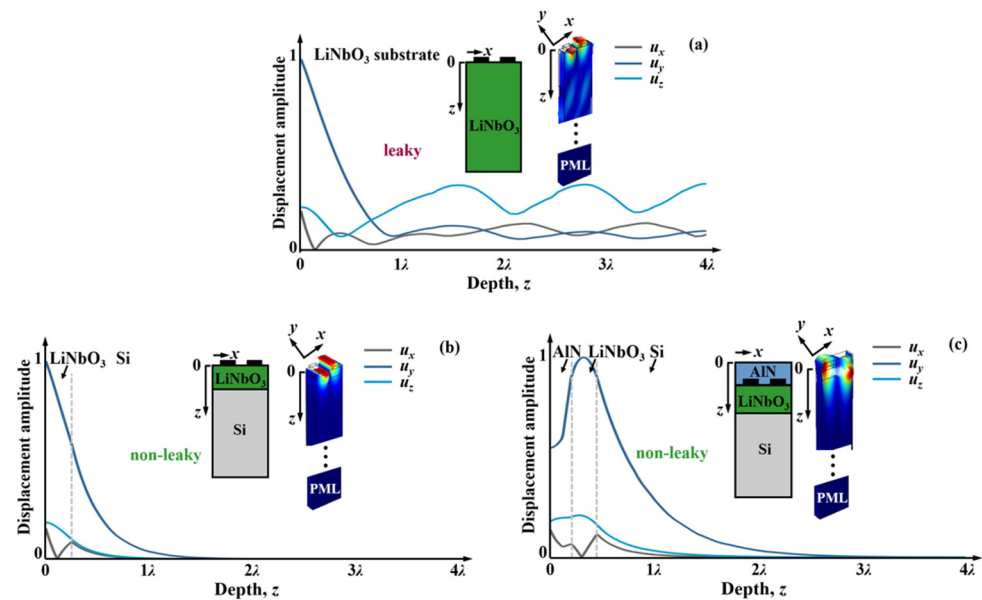
**Table 1.** Symbols used in this paper.

| Symbol               | Definition                             |
|----------------------|----------------------------------------|
| $Q$                  | Quality Factor                         |
| $k_{\text{eff}}^2$   | Electromechanical Coupling Coefficient |
| $\lambda$            | Acoustic Wavelength                    |
| $f_s$                | Series-frequency                       |
| $u_x$                | $x$ -direction displacement            |
| $u_y$                | $y$ -direction displacement            |
| $u_z$                | $z$ -direction displacement            |
| $h_{\text{LiNbO}_3}$ | The thickness of LiNbO <sub>3</sub>    |
| $h_{\text{AlN}}$     | The thickness of AlN                   |
| $S_0$ mode           | The lowest symmetric mode              |
| $v_{p,o}$            | Open phase velocity                    |
| TCF                  | Temperature coefficients of frequency  |
| TCV                  | Temperature coefficients of velocity   |

## 2. Substrate Leakage

Figure 1 depicts the FEM-simulated mode shapes of the SH wave propagating in LiNbO<sub>3</sub> substrate, LiNbO<sub>3</sub>/Si layered substrate, and AlN/LiNbO<sub>3</sub>/Si layered substrate. Perfect-matched-layer (PML) physics is assigned to bottom layers of the 3D unit cell models to simulate the substrate that is too thick, comparing it to wavelengths to generate wave reflections from its bottom. The periodic conditions are applied to both  $x$  (perpendicular to IDT fingers) and  $y$  (in parallel with IDT fingers) directions so that the basic semi-infinite plane condition is assumed for the wave propagation. The material con-

stants are from [14–17] and are listed in Table 2. In the structures shown,  $h_{\text{LiNbO}_3}/\lambda = 0.25$ ,  $h_{\text{AlN}}/\lambda = 0.2$  are assumed;  $8\% \lambda$ -thick aluminum (Al) is used as IDT electrodes here and throughout the paper.



**Figure 1.** Comparison of simulated displacement amplitudes of (a) LiNbO<sub>3</sub> substrate, (b) LiNbO<sub>3</sub>/Si, and (c) AlN/ LiNbO<sub>3</sub>/Si for the SH wave. The insets are the mode shapes at antiresonances simulated with periodic structures using FEM simulation ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ,  $h_{\text{AlN}}/\lambda = 0.2$ ,  $h_{\text{IDT,Al}}/\lambda = 0.08$  are used in the plots).

**Table 2.** LiNbO<sub>3</sub>, AlN, Si, and Al material constants used in the simulations [14–16].

| Parameter               | Symbol            | LiNbO <sub>3</sub> [14] | AlN [15] | Si [16] | Al [16] | Units                   |
|-------------------------|-------------------|-------------------------|----------|---------|---------|-------------------------|
| Stiffness constants     | $C_{11}^E$        | 198.39                  | 345      |         | 111     | (GPa)                   |
|                         | $C_{12}^E$        | 54.72                   | 125      |         | 59      |                         |
|                         | $C_{13}^E$        | 65.13                   | 120      |         | 59      |                         |
|                         | $C_{14}^E$        | 7.88                    | –        | 170     | –       |                         |
|                         | $C_{33}^E$        | 227.90                  | 395      |         | 111     |                         |
|                         | $C_{44}^E$        | 59.65                   | 118      |         | 26      |                         |
|                         | $C_{66}^E$        | 71.84                   | 110      |         | 26      |                         |
| Density                 | $\rho$            | 4628                    | 3260     | 2329    | 2700    | (kg/m <sup>3</sup> )    |
| Piezoelectric constants | $e_{15}$          | 3.69                    | −0.48    | –       | –       | (C/m <sup>2</sup> )     |
|                         | $e_{22}$          | 2.42                    | –        | –       | –       |                         |
|                         | $e_{31}$          | 0.30                    | −0.58    | –       | –       |                         |
|                         | $e_{33}$          | 1.77                    | 1.55     | –       | –       |                         |
| Dielectric constants    | $\epsilon_{11}^S$ | 45.6                    | 8.0      | 11.7    | 1       | (10 <sup>−11</sup> F/m) |
|                         | $\epsilon_{33}^S$ | 26.3                    | 9.5      | 11.7    | 1       |                         |

As shown in Figure 1a, the shear component in YX-LiNbO<sub>3</sub> substrate still concentrates at the surface, but strong leakage results from coupling to the slow shear bulk acoustic wave and mechanically propagates down obliquely, as shown in  $u_z$  and  $u_x$ . The lower-case coordinate  $x$  is the propagation direction proportional to IDT,  $y$  is the transversal direction parallel to IDT, and  $z$  the direction down into substrate. By bonding the high-velocity Si

substrate to the sub-wavelength YX-LiNbO<sub>3</sub>, the SH wave in LiNbO<sub>3</sub>/Si (Figure 1b) no longer couples with the bulk mode and leaks into the substrate since the bulk velocity is higher than the SH mode on surface. After adding an AlN coating layer, the SH mode still concentrates in the LiNbO<sub>3</sub> piezoelectric layer and minimizes the leaky component into the Si substrate (Figure 1c).

### 3. Propagation Characteristics of SH Wave in LiNbO<sub>3</sub>/Si

The  $v_p$  and  $k_{\text{eff}}^2$  of the SH waves propagating in the single and layered piezoelectric substrates can be theoretically calculated using numerical analysis—Adler’s matrix approach [17] or FEM [18]. The material constants for both the calculation and FEM simulation are also listed in Table 2. The numerically calculated propagation characteristics are checked with FEM simulation and agreed well with the FEM results. In the FEM simulation, the model is a 3D building-block cell with periodic boundary conditions (BCs) on both  $x$ - and  $y$ - directions. All the  $k_{\text{eff}}^2$  are derived from series-resonance frequency ( $f_s$ ) and parallel-resonance frequency ( $f_p$ ) using the IEEE standard definition of the device electromechanical coupling [19]:

$$k_{\text{eff}}^2 = \frac{\pi f_s}{2 f_p} \left[ \tan\left(\frac{\pi f_s}{2 f_p}\right) \right]^{-1}. \quad (1)$$

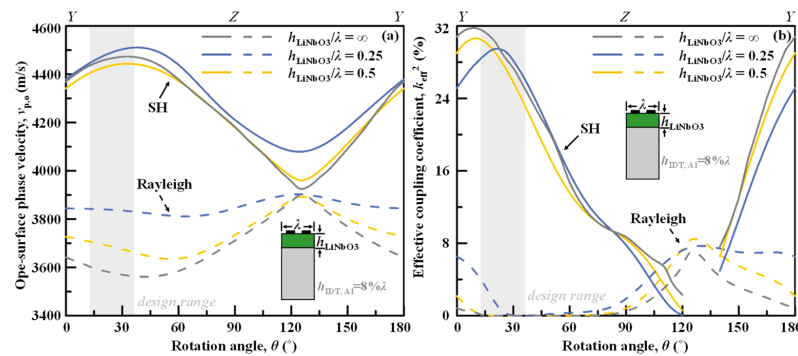
Comparing to the intrinsic coupling coefficient ( $k_{\text{intr}}^2$ ) derived from the difference from the open- and metallized-surface  $v_p$ :

$$k_{\text{intr}}^2 = \frac{v_{p,o}^2 - v_{p,m}^2}{v_{p,o}^2} \quad (2)$$

the device-level  $k_{\text{eff}}^2$  yields close values to the  $k_{\text{intr}}^2$  and considers the electric field more accurately. The differences of these two definitions of couplings are discussed and compared in detail in Figure 2 of the reference [18]. Despite the similarity for a standard device, the impact of the actual electrode cross-sectional shape and coverage ratio can be considered in the  $k_{\text{eff}}^2$  derivation but not  $k_{\text{intr}}^2$ , so the  $k_{\text{eff}}^2$  evaluation offers better accuracy and potential for the future device optimization. As a result, the device-level coupling coefficient  $k_{\text{eff}}^2$  is utilized throughout the analysis of this work.

#### 3.1. Cut Angle

As the propagation loss is no longer the main concern and dictates the cut-angle selection for the nonleaky SH wave in bonded wafers, the optimal cut angle can be chosen to optimize  $v_p$  and  $k_{\text{eff}}^2$ . Figure 2a,b depicts the open-surface phase velocities  $v_{p,o}$  and  $k_{\text{eff}}^2$  for LiNbO<sub>3</sub>/Si across all rotation angles  $\theta$  from the YX-LiNbO<sub>3</sub> with varied thicknesses of LiNbO<sub>3</sub> for both the SH main mode and the Rayleigh spurious mode.



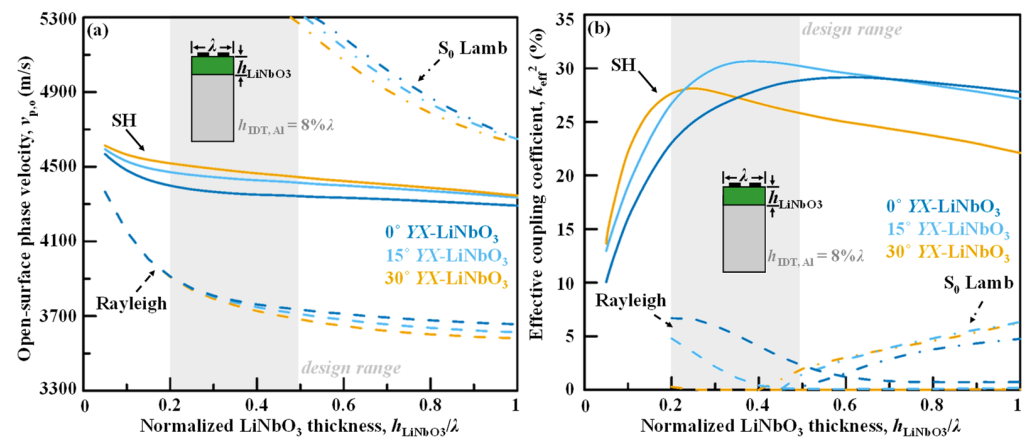
**Figure 2.** Simulated (a) open-surface phase velocities  $v_{p,o}$  and (b) effective coupling coefficient  $k_{\text{eff}}^2$  for LiNbO<sub>3</sub>/Si across all rotation angles from the YX-LiNbO<sub>3</sub> with varied thicknesses of LiNbO<sub>3</sub> for the SH main mode and Rayleigh spurious mode.

The impact of the rotation angle on the propagation characteristics of SH mode in LiNbO<sub>3</sub>/Si layered substrate is similar to on the LiNbO<sub>3</sub> substrate [20], as depicted in Figure 2a. Fortunately, a low rotation angle from YX-LiNbO<sub>3</sub> enables high  $v_{p,o}$ , large  $k_{\text{eff}}^2$  for the SH main mode, and low  $k_{\text{eff}}^2$  for Rayleigh mode simultaneously. Therefore, the design range of  $\theta$  is 10–40° for the LiNbO<sub>3</sub>/Si-based nonleaky SH wave devices for the high frequency, wide band, and clean spectrum, respectively.

In Figure 2b, it can also be noted that  $h_{\text{LiNbO}_3} = 0.25\lambda$  enables higher  $v_{p,o}$  than  $h_{\text{LiNbO}_3} = 0.5\lambda$  of LiNbO<sub>3</sub>/Si or LiNbO<sub>3</sub> substrate, and the optimized rotation angle also shifts up a bit for the optimum  $k_{\text{eff}}^2$ . These indicate weak dispersion in the layered substrate due to the sub-wavelength-thick piezo thin film.

### 3.2. Dispersion and Spurious Modes

As shown in Figure 3a,b, the dispersive curves of the  $v_{p,o}$ 's and  $k_{\text{eff}}^2$ 's of the SH main mode, Rayleigh spurious mode, and S<sub>0</sub> Lamb mode spurious mode propagating in the LiNbO<sub>3</sub>/Si bonded structure with varied rotation angle of YX-LiNbO<sub>3</sub> are presented. Due to the sub-wavelength thick piezo-layer structure, the SH mode and Rayleigh mode show weak dispersive characteristics in the phase velocities. The S<sub>0</sub> Lamb wave, however, shows even stronger dispersion due to its plate-wave type whose characteristics are usually impacted a lot by the piezoelectric-layer thickness normalized to wavelength. Although varying LiNbO<sub>3</sub> thickness does not move the Rayleigh spurious mode away from the SH main mode in frequency, engineering the LiNbO<sub>3</sub> thickness does effectively keep the Lamb modes distant in frequency from the SH mode. Luckily, when the  $h_{\text{LiNbO}_3} < 0.5\lambda$ , the closest Lamb mode S<sub>0</sub> mode would be 20% higher in frequency than the SH main mode, which makes a distance of at least 500 MHz if the SH passband is at 2.5 GHz.

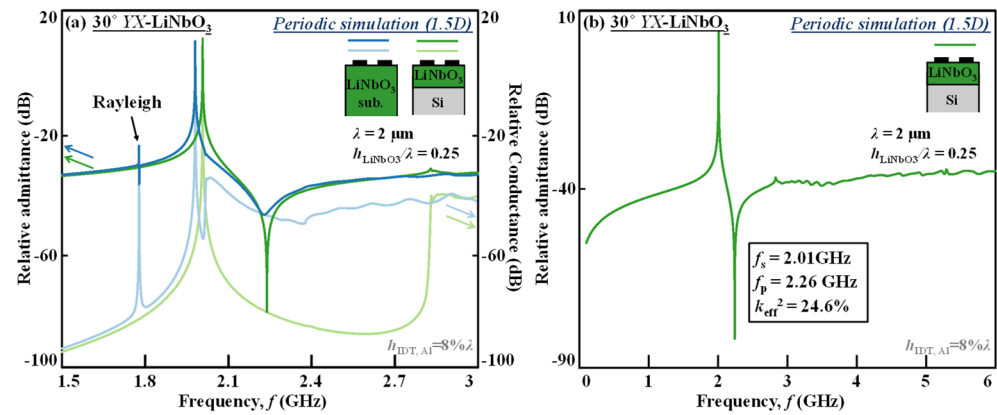


**Figure 3.** Calculated dispersion curves of (a) open-surface phase velocities  $v_{p,o}$  and (b) effective coupling coefficient  $k_{\text{eff}}^2$  for the LiNbO<sub>3</sub>/Si with varied rotation angle of YX-LiNbO<sub>3</sub>.

The dispersive characteristics in  $k_{\text{eff}}^2$  is stronger than in  $v_{p,o}$  for the SH mode, as shown in Figure 3b. In other words, the change of  $k_{\text{eff}}^2$  for SH mode with  $h_{\text{LiNbO}_3}$  is more obvious than that of  $v_{p,o}$ . In order to achieve a high  $k_{\text{eff}}^2$ , the LiNbO<sub>3</sub> cannot be too thin or too thick and the design range is preferred to be  $>0.2\lambda$  and  $<0.5\lambda$ . In addition, the Rayleigh and S<sub>0</sub> Lamb spurious modes can also be suppressed by choosing the LiNbO<sub>3</sub> thickness and cut-angle combination smartly. For the S<sub>0</sub> Lamb mode, the case is simpler since its  $k_{\text{eff}}^2$  will lower at smaller LiNbO<sub>3</sub> thicknesses under different LiNbO<sub>3</sub> cut angle, and the design range of  $h_{\text{LiNbO}_3} < 0.5\lambda$  fortunately happens to be able to suppress the S<sub>0</sub> Lamb modes. As a contrary, the LiNbO<sub>3</sub> thickness and rotation angle have to be optimized together for the Rayleigh mode, and a slightly larger rotation angle is preferred for the  $0.2\lambda < h_{\text{LiNbO}_3} < 0.5\lambda$  design range, such as 30° YX-LiNbO<sub>3</sub>.

### 3.3. Frequency Response

Figure 4a,b show the FEM-simulated narrow-band response compared to LiNbO<sub>3</sub> substrate and wide-band response with periodic structure, which is a 1.5-dimension (1.5 D) model based on LiNbO<sub>3</sub>/Si with 30° YX-LiNbO<sub>3</sub> and  $h_{\text{LiNbO}_3}/\lambda = 0.25$ . By the 1.5D model we assume an infinite number of IDT fingers ( $NF$ ) and infinite aperture lengths, but the stack setup in  $z$  direction is fully considered (1D), as well as the IDT duty factor ( $DF = \text{finger width/pitch}$ ) and IDT shape in periodicity (0.5D).



**Figure 4.** FEM-simulated (a) narrow-band response compared to LiNbO<sub>3</sub> substrate, and (b) wide-band response of the SH resonators with periodic structure (1.5D model) based on LiNbO<sub>3</sub>/Si with 30° YX LiNbO<sub>3</sub> and  $h_{\text{LiNbO}_3}/\lambda = 0.25$ .

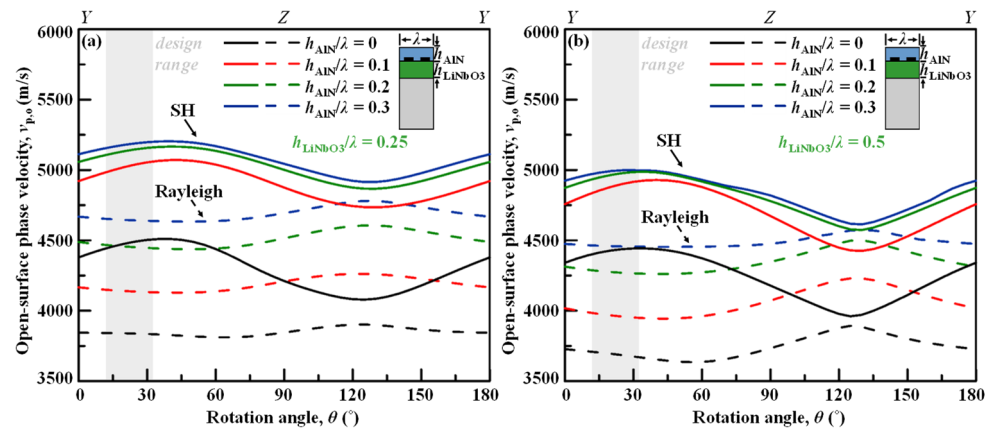
Comparing the conductance and admittance curves of the SH modes in LiNbO<sub>3</sub> substrate and LiNbO<sub>3</sub>/Si in Figure 4a, it is clearly seen that in LiNbO<sub>3</sub> substrate, as the bulk wave velocity is lower than SH wave, the antiresonance is distorted with low- $Q$ , and from the conductance curve it could be observed that the wave cannot be effectively reflected in the stopband as well. On the contrary, for LiNbO<sub>3</sub>/Si stack, the parallel resonance features a very sharp response and the conductance level is very deep around the  $f_p$  and throughout the stopband thanks to the minimal bulk radiation, again indicating the ultra-low propagation loss and the fact of nonleaky characteristics.

In addition, for the LiNbO<sub>3</sub>/Si and at this LiNbO<sub>3</sub> cut angle and LiNbO<sub>3</sub> layer thickness designed to lower the Rayleigh  $k_{\text{eff}}^2$  to near-zero, the narrow-band response (Figure 4a) is clean from the Rayleigh mode, which presents in the response based on LiNbO<sub>3</sub> substrate. On the other hand, since the LiNbO<sub>3</sub> is thin enough, the wide-band response of the LiNbO<sub>3</sub>/Si resonator also shows an extremely clean spectrum from 0 to 6 GHz.

## 4. Propagation Characteristics of SH Wave in AlN/LiNbO<sub>3</sub>/Si

### 4.1. Cut Angle

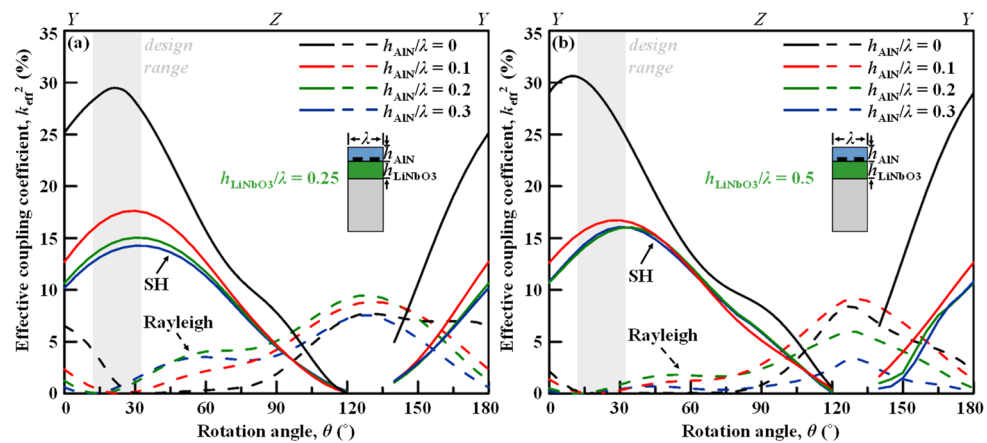
Figure 5a,b depict the open-surface phase velocities  $v_{p,o}$  for varied normalized thicknesses of AlN overlay layer on top of the IDT transducers sitting on LiNbO<sub>3</sub>/Si and the piezo-layer is across all rotation angles from the YX-LiNbO<sub>3</sub> with  $h_{\text{LiNbO}_3}/\lambda = 0.25$  and  $h_{\text{LiNbO}_3}/\lambda = 0.5$ , respectively. The  $c$ -axis-oriented AlN material constants are from literature [15] and listed in Table 2. The nonleaky SH wave propagating in the AlN/LiNbO<sub>3</sub>/Si stack shows a similar trend to that in the LiNbO<sub>3</sub>/Si layered stack. For both LiNbO<sub>3</sub> thickness cases, the phase velocity can be effectively enhanced by the AlN overlay, and the improvement converges when  $h_{\text{AlN}}$  is larger than  $0.2\lambda$ . The phase velocities of the SH modes in Figure 5a with  $h_{\text{LiNbO}_3}/\lambda = 0.25$  are in general larger than the case in Figure 5b with  $h_{\text{LiNbO}_3}/\lambda = 0.5$ . As can be observed in Figure 5a, with  $h_{\text{LiNbO}_3}/\lambda = 0.25$  and for  $\theta$  between 20° and 80°, the  $v_{p,o}$  can be as high as above 5000 m/s thanks to the AlN coating with  $h_{\text{AlN}} > 0.2\lambda$ .



**Figure 5.** Calculated open phase velocities  $v_{p,o}$  for varied thicknesses of AlN overlay layer on LiNbO<sub>3</sub>/Si across all rotation angles from the YX-LiNbO<sub>3</sub> with (a)  $h_{\text{LiNbO}_3}/\lambda = 0.25$ , and (b)  $h_{\text{LiNbO}_3}/\lambda = 0.5$ .

Furthermore, the Rayleigh mode in the case of  $h_{\text{LiNbO}_3}/\lambda = 0.25$  are less coupled with the SH mode at a high rotation angle of around  $128^\circ$ , and also less perturbed by  $\theta$  than the case of  $h_{\text{LiNbO}_3}/\lambda = 0.5$ . At low  $\theta < 30^\circ$ ; however, the Rayleigh spurious mode is slightly closer to the SH mode in the case of  $h_{\text{LiNbO}_3}/\lambda = 0.25$  than in the thicker case, which is in a similar trend with Figure 3a.

Figure 6a and b depict the effective coupling coefficient  $k_{\text{eff}}^2$  for varied thicknesses of AlN overlay layer on LiNbO<sub>3</sub>/Si across all rotation angles from the YX LiNbO<sub>3</sub> with  $h_{\text{LiNbO}_3}/\lambda = 0.25$  and  $h_{\text{LiNbO}_3}/\lambda = 0.5$ , respectively. Although the AlN overlay apparently lowers the  $k_{\text{eff}}^2$ , the degraded  $k_{\text{eff}}^2$  would still be more than enough and much larger than the current technologies. Moreover, the reduction in  $k_{\text{eff}}^2$  would converge when  $h_{\text{AlN}}$  is larger than  $0.2\lambda$ . For both LiNbO<sub>3</sub> thickness cases, and for cut angles between  $0^\circ$  and  $60^\circ$ , the  $k_{\text{eff}}^2$  can be as high as above 11%. Comparing two LiNbO<sub>3</sub> thicknesses, the peak  $k_{\text{eff}}^2$  of the SH mode in AlN/LiNbO<sub>3</sub>/Si across a wide rotation-angle range are at similar level.

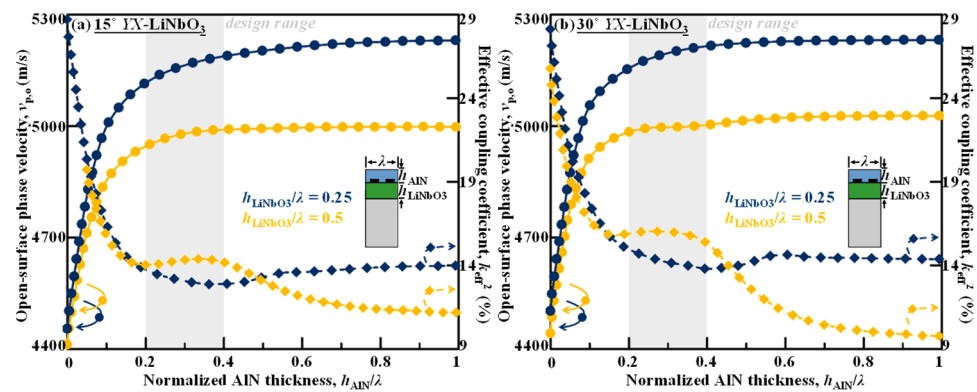


**Figure 6.** Calculated coupling coefficient  $k_{\text{eff}}^2$  for varied thicknesses of AlN overlay layer on LiNbO<sub>3</sub>/Si across all rotation angles from the YX-LiNbO<sub>3</sub> with (a)  $h_{\text{LiNbO}_3}/\lambda = 0.25$ , and (b)  $h_{\text{LiNbO}_3}/\lambda = 0.5$ .

It is also interesting to note that at  $\theta \sim 10^\circ$ – $30^\circ$ , the  $k_{\text{eff}}^2$  of SH mode is maximized and at the same time the  $k_{\text{eff}}^2$  of Rayleigh mode is minimized, where the Rayleigh spurious mode can be suppressed in the nonleaky SH SAW resonator or filter. With AlN overlays, the optimized cut angle for Rayleigh mode elimination shifts down a bit. The optimal cut-angle design range would be of  $10^\circ$ – $30^\circ$  for simultaneously achieving high  $v_{p,o}$  and large  $k_{\text{eff}}^2$  for the SH mode, as well as low- $k_{\text{eff}}^2$  for Rayleigh mode.

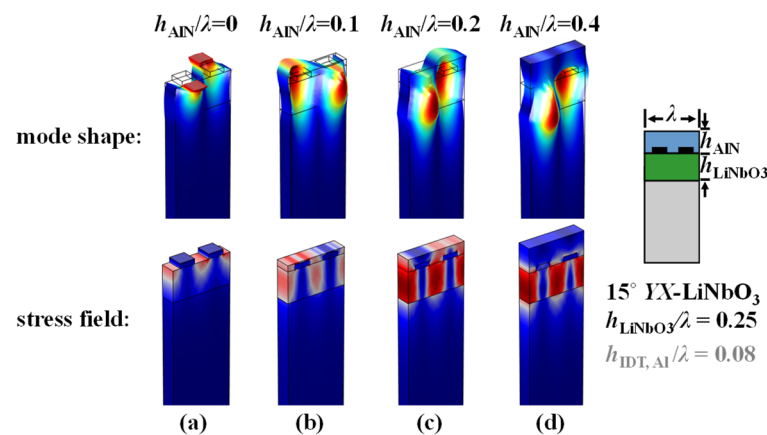
#### 4.2. Trade-Offs between $v_{p,o}$ and $k_{eff}^2$

The trade-offs between the  $v_{p,o}$  and  $k_{eff}^2$  by varying AlN thickness are compared for the nonleaky SH wave propagating in AlN/LiNbO<sub>3</sub>/Si with two different rotation angles of the piezoelectric LiNbO<sub>3</sub>, as presented in Figure 7a,b. It can be noted that both the  $v_{p,o}$  and  $k_{eff}^2$  saturate when  $h_{AlN} > 0.4\lambda$ . For both 15° YX-LiNbO<sub>3</sub> and 30° YX-LiNbO<sub>3</sub>, the  $v_{p,o}$  is much higher for the case of  $h_{LiNbO_3} = 0.25\lambda$  than  $h_{LiNbO_3} = 0.5\lambda$ , and the  $k_{eff}^2$  is also slightly higher for the thinner case. At  $\theta = 15^\circ$ , the saturated  $v_{p,o}$  is as high as 5280 m/s when  $h_{LiNbO_3} = 0.25\lambda$ ; at  $\theta = 30^\circ$ , the saturated  $v_{p,o}$  is 5240 m/s when  $h_{LiNbO_3} = 0.25\lambda$ . The preferred AlN thickness design range would be between  $0.2\lambda$  and  $0.4\lambda$  right before the convergence in order to avoid additional mass loading on the device coupling.



**Figure 7.** Trade-offs between the open-surface phase velocities  $v_{p,o}$  and coupling coefficient  $k_{eff}^2$  by varying AlN thickness for the SH wave propagating in AlN/LiNbO<sub>3</sub>/Si based on (a) 15° YX-LiNbO<sub>3</sub> and (b) 30° YX-LiNbO<sub>3</sub> with  $h_{LiNbO_3}/\lambda = 0.25$  and  $h_{LiNbO_3}/\lambda = 0.5$ .

Figure 8 depicts the displacement field as well as the first principal stress field of the nonleaky SH mode on the AlN/LiNbO<sub>3</sub>/Si with increasing AlN normalized thicknesses. It is most obvious that the mechanical fields become more penetrated and uniform when AlN becomes thicker. It is also intriguing to note that when the AlN layer is thicker than  $0.4\lambda$ , the vibration becomes off the surface and concentrated in the highly piezo LiNbO<sub>3</sub> layer; the AlN film then starts to be free of the mechanical vibration and transduction, indicating a stable mechanical-loading effect only instead of wave perturbation.



**Figure 8.** FEM-simulated mode shapes and the first principal stress field of the nonleaky SH mode on the AlN/LiNbO<sub>3</sub>/Si substrate stack with (a)  $h_{AlN}/\lambda = 0$ , (b)  $h_{AlN}/\lambda = 0.1$ , (c)  $h_{AlN}/\lambda = 0.2$ , and (d)  $h_{AlN}/\lambda = 0.4$ .

Both the saturated values of  $v_{p,o}$  and  $k_{eff}^2$  are larger in the case of  $h_{LiNbO_3} = 0.25\lambda$  compared to  $h_{LiNbO_3} = 0.5\lambda$  for either 15° YX-LiNbO<sub>3</sub> or 30° YX-LiNbO<sub>3</sub>. Note at for

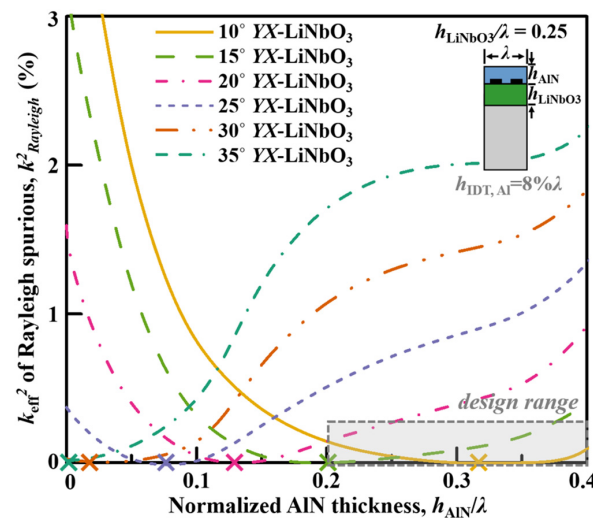
the 15° YX-LiNbO<sub>3</sub> case, 0.5λ-thick LiNbO<sub>3</sub> yields larger  $k_{\text{eff}}^2$  than 0.25λ-thick LiNbO<sub>3</sub> when AlN overlay is not applied and  $h_{\text{AlN}} = 0$ , which can also be observed from Figure 4b. However, even with slight AlN overlay, the  $k_{\text{eff}}^2$  of 0.25λ-thick LiNbO<sub>3</sub> becomes similar or larger. As a result, for both rotation-angle cases, the 0.25λ-thick LiNbO<sub>3</sub> enables much higher  $v_{p,o}$  and similar  $k_{\text{eff}}^2$ .

When  $h_{\text{LiNbO}_3} = 0.25\lambda$ , the  $v_{p,o}$  can be effectively boosted from 4420 m/s to 5280 m/s, showing a near 20% increase when  $h_{\text{AlN}}$  is up to  $>0.4\lambda$ . Although the  $k_{\text{eff}}^2$  is decreased by increasing  $h_{\text{AlN}}$ , the absolute value is still above 14% even with a large  $h_{\text{AlN}}$ , which is sufficient for most commercial bandwidths, thanks to the super-large intrinsic material electromechanical coupling  $K^2$  of the low-angle-rotated YX-LiNbO<sub>3</sub>.

#### 4.3. Rayleigh Spurious

With the ability of high electromechanical coupling, the Rayleigh mode performs as the major spurious mode for most SH main-mode devices. In addition to the phase velocities of the Rayleigh mode always being very close to the SH mode, the Rayleigh spurious mode could generate prominent passband notches and near-band spikes for the SH wave filters, and pose severe risks for the application of the nonleaky SH waves. Therefore, the suppression of the Rayleigh spurious mode is highly desirable.

Figure 9 depicts the simulated  $k_{\text{eff}}^2$  of the Rayleigh spurious mode versus AlN thicknesses for the AlN/LiNbO<sub>3</sub>/Si with different rotation angle and  $h_{\text{LiNbO}_3}/\lambda = 0.25$ . While the 30° and 35° rotation angles enable near-zero  $k_{\text{eff}}^2$  of the Rayleigh mode, when AlN overlay becomes thicker, the preferred rotation angle is smaller for the low  $k_{\text{eff}}^2$  of the Rayleigh mode. Or, in other words, for different rotation angles of the LiNbO<sub>3</sub> layer, the optimized AlN thicknesses for zero-coupling Rayleigh mode are varied: for relatively lower rotation angle, the optimized AlN thickness would be large to diminish the Rayleigh mode.



**Figure 9.** Simulated  $k_{\text{eff}}^2$  of the Rayleigh spurious mode versus AlN thicknesses for the AlN/LiNbO<sub>3</sub>/Si with different rotation angles and  $h_{\text{LiNbO}_3}/\lambda = 0.25$ . The cross labels mark the AlN thicknesses that enables full suppression of the Rayleigh mode.

As concluded in the previous section, 0.2λ–0.4λ thick AlN overlay is preferred for enabling the large velocity and  $k_{\text{eff}}^2$  level at the same time. The optimized cut angle for the near-zero coupling of the Rayleigh spurious mode would be between 10° and 15° YX-LiNbO<sub>3</sub>, as shown in the yellow and green curves as examples inside the design range marked in Figure 9. Again, from the green and blue curves in Figure 6a, it can be found that 15° YX-LiNbO<sub>3</sub> with 0.2λ AlN enables larger  $k_{\text{eff}}^2$  of the main mode than 10° YX-LiNbO<sub>3</sub> with 0.3λ AlN. As a result, 15° YX-LiNbO<sub>3</sub> with 0.2λ AlN can be chosen for a high suppression of the Rayleigh spurious mode, as well as enabling large  $v_p$  and high  $k_{\text{eff}}^2$  for the main SH main mode simultaneously.

#### 4.4. Improvement of TCF

In addition, without a careful design of the substrate, the layered SH potentially has spurious responses in the out-of-band frequencies (Lamb modes) and near-band frequencies. This paper focuses on the design of layered substrate not only to optimize its narrow-band characteristics— $f$ ,  $Q$ ,  $k_{\text{eff}}^2$ , temperature coefficient of frequency (TCF)—but also for eliminating the out-of-band spurious responses.

The TCF performance measuring the thermal stability of a resonator is set by the temperature dependence of phase velocity and the thermal-expansion coefficient of the wave along the propagation direction. The first-order TCF's for the series resonance ( $TCF_{s,1st}$ ) and parallel resonance ( $TCF_{p,1st}$ ) are calculated as

$$TCF_{s,1st} = \frac{1}{f_s} \frac{\partial f_s}{\partial T} = \frac{1}{v_{p,SC}} \frac{\partial v_{p,SC}}{\partial T} - \alpha_x, \quad (3)$$

$$TCF_{p,1st} = \frac{1}{f_p} \frac{\partial f_p}{\partial T} = \frac{1}{v_{p,OC}} \frac{\partial v_{p,OC}}{\partial T} - \alpha_x, \quad (4)$$

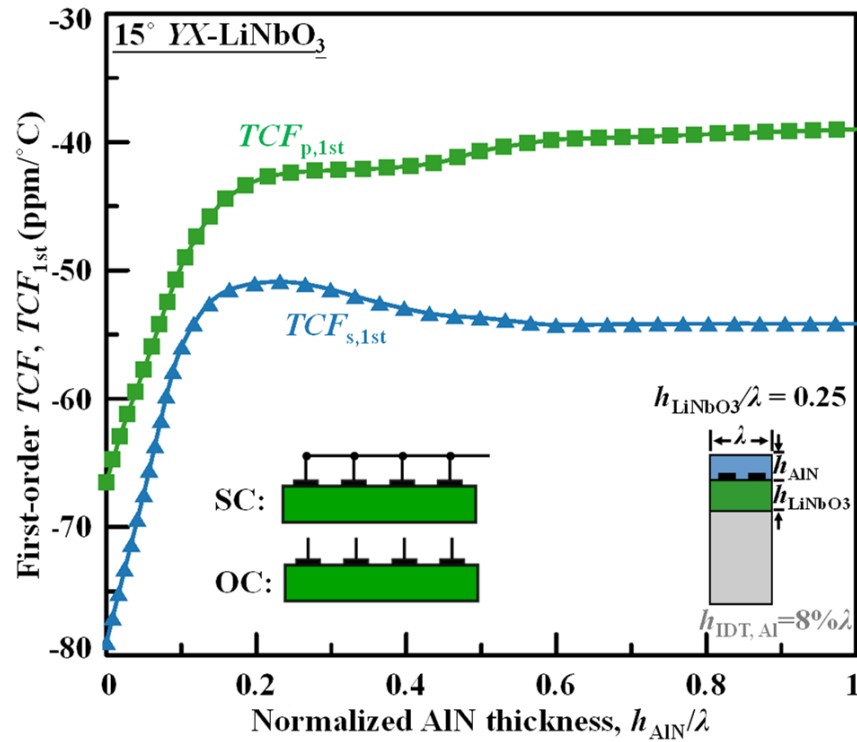
where  $v_{p,SC}$  and  $v_{p,OC}$  refer to the phase velocities under short-circuited (SC) and open-circuited (OC) grating BCs, shown in the inset of FIG 10. From the coupling-of-modes (COM) theory, these BCs corresponds to the  $f_s$  and  $f_p$ , respectively. Their temperature dependence  $\partial/\partial T$  is calculated from the temperature coefficients of stiffness constants, temperature coefficients of piezoelectric constants, and temperature coefficients of permittivity of LiNbO<sub>3</sub>, AlN, Si, and Al listed in Table 3. The  $\alpha_x$  corresponds to the thermal-expansion coefficient of the substrate in the wave-propagation direction  $x$ , also listed in Table 3. Since the Si substrate is much thicker than the LiNbO<sub>3</sub> and AlN, the effect of thermal expansion is limited by the clamping substrate Si, and its  $\alpha_{11}$  of 2.6 ppm/°C from literature [19] is used herein for the derivation.

**Table 3.** Temperature coefficients of material constants of LiNbO<sub>3</sub>, AlN, Si, and Al used in the simulations [15,16,21].

| Parameter                                                   | Symbol           | LiNbO <sub>3</sub> [21] | AlN [15] | Si [16] | Al [15] | Units                   |
|-------------------------------------------------------------|------------------|-------------------------|----------|---------|---------|-------------------------|
| Temperature coefficients of stiffness constants (1st order) | $Tc_{11}$        | −174                    | −37      | −63     | −590    | (10 <sup>−6</sup> 1/°C) |
|                                                             | $Tc_{12}$        | −252                    | −1.8     |         | −80     |                         |
|                                                             | $Tc_{13}$        | −159                    | −1.8     |         | −80     |                         |
|                                                             | $Tc_{14}$        | −214                    | −        |         | −       |                         |
|                                                             | $Tc_{33}$        | −153                    | −65      |         | −590    |                         |
|                                                             | $Tc_{44}$        | −204                    | −50      |         | −520    |                         |
|                                                             | $Tc_{66}$        | −143                    | −57      |         | −520    |                         |
| Temperature coefficients of piezoelectric constants         | $Te_{15}$        | 147                     | −        | −       | −       | (10 <sup>−6</sup> 1/°C) |
|                                                             | $Te_{22}$        | 79                      |          |         |         |                         |
|                                                             | $Te_{31}$        | 221                     |          |         |         |                         |
|                                                             | $Te_{33}$        | 887                     |          |         |         |                         |
| Temperature coefficients of permittivity                    | $T\epsilon_{11}$ | 323                     | −        | −       | −       | (10 <sup>−6</sup> 1/°C) |
|                                                             | $T\epsilon_{33}$ | 627                     |          |         |         |                         |
| Thermal-expansion coefficients                              | $\alpha_{11}$    | 15.4                    | 5.27     | 2.6     | 18      | (10 <sup>−6</sup> 1/°C) |
|                                                             | $\alpha_{33}$    | 7.5                     | 4.15     | 2.6     | 18      |                         |

Figure 10 shows the calculated  $TCF_{s,1st}$  and  $TCF_{p,1st}$  by varying the AlN thickness for the nonleaky SH waves propagating in AlN/LiNbO<sub>3</sub>/Si with the 0.25 $\lambda$ -thick 15° YX-LiNbO<sub>3</sub> optimized from the previous analysis. Although AlN also becomes softer

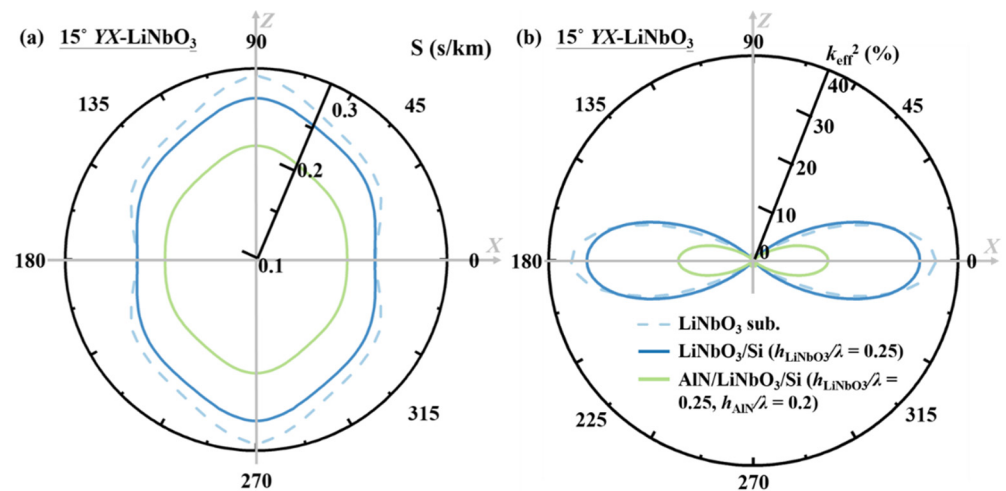
(contributing to  $TCV$ ) and larger (contributing to  $\alpha$ ) when temperature rises, its  $TCF$  absolute value is much lower than  $\text{LiNbO}_3 \sim -26 \text{ ppm}/^\circ\text{C}$ . Thus, the thicker  $\text{AlN}$  can reduce the thermal dependence of the phase velocity for the SH wave traveling in the composite structure. The  $TCF_{p,1st}$  is always lower than  $TCF_{s,1st}$  due to the positive  $T_{e15}$  and  $T_{e22}$  of  $\text{LiNbO}_3$ ; at a high temperature,  $k_{\text{eff}}^2$  would increase slightly.



**Figure 10.** Calculated  $TCF_{s,1st}$  and  $TCF_{p,1st}$  by varying  $\text{AlN}$  thickness for the SH wave propagating in  $\text{AlN}/\text{LiNbO}_3/\text{Si}$ . The inset depicts the short-circuited and open-circuited grating conditions, corresponding to resonance and parallel resonance, respectively.

#### 4.5. Slowness Curve and Propagation Direction

Although the propagation direction can be lithographically controlled in most cases along the X direction (all the previous analysis assumes the X propagation direction), the polar plots of propagating characteristics versus propagation direction can be good indicators for understanding the wave properties as well as fostering the device design [20]. Figure 11a,b show the slowness ( $S$ ) curve and the  $k_{\text{eff}}^2$  of the SH wave versus different propagation directions on the  $\text{LiNbO}_3$  substrate,  $\text{LiNbO}_3/\text{Si}$  ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ), and  $\text{AlN}/\text{LiNbO}_3/\text{Si}$  ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ,  $h_{\text{AlN}}/\lambda = 0.2$ ). The slowness curve for the  $\text{LiNbO}_3$  substrate shows a concave feature, whereas for the  $\text{LiNbO}_3/\text{Si}$  and  $\text{AlN}/\text{LiNbO}_3/\text{Si}$  stacks it is nearly straight near the  $x$ -axis, indicating minimal diffraction of the nonleaky SH wave. Usually, for a well-guided wave with convex slowness curves, a faster region is required at the lateral ends to guide the wave, and for the concave case there might be lateral leakage to the fast regions. For the “straight” type [3], the IDT gap region design would be different and less sensitive to the concave or convex cases. In addition, from Figure 11a, the phase  $v_p$ ’s is largely enhanced in all propagation directions after adding the  $\text{AlN}$  overlay.



**Figure 11.** Calculated (a) slowness curve; (b) effective coupling coefficient  $k_{\text{eff}}^2$  of the SH wave versus different propagation direction on the  $15^\circ$  YX-LiNbO<sub>3</sub> substrate, LiNbO<sub>3</sub>/Si ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ), and AlN/ LiNbO<sub>3</sub>/Si ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ,  $h_{\text{AlN}}/\lambda = 0.2$ ).

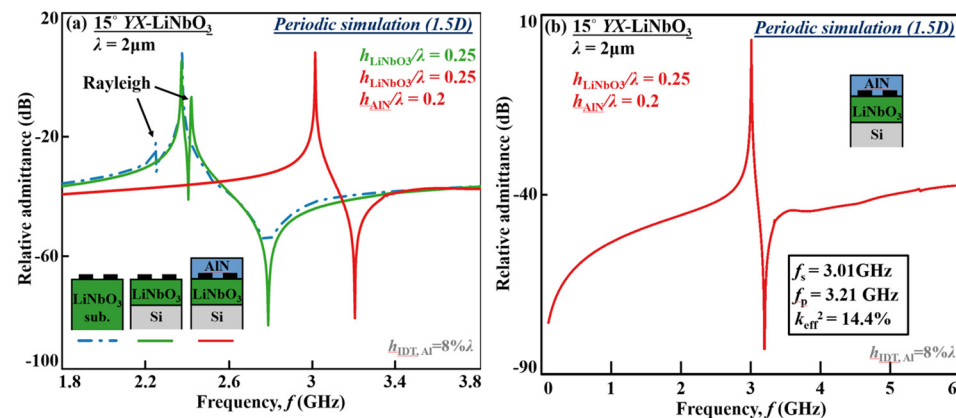
In Figure 11b, the  $k_{\text{eff}}^2$  decreases drastically when the propagation direction deviates from the X-axis. In propagation directions close to X, the  $k_{\text{eff}}^2$  is slightly reduced from LiNbO<sub>3</sub> substrate to the LiNbO<sub>3</sub>/Si nonleaky stack (agreeing with Figure 2b in the X axis case); in propagation directions close to Z, the  $k_{\text{eff}}^2$  is very slightly improved from LiNbO<sub>3</sub> substrate to the LiNbO<sub>3</sub>/Si bonded structure. After adding the AlN overlay on top of the transducer, the  $k_{\text{eff}}^2$  reduces drastically due to the mechanical loading effect, and in the X direction the  $k_{\text{eff}}^2$  falls to between 10% and 15%, which is still more than enough for the advanced LTE bandwidth specification and most of the 5G NR bands.

In summary, the optimized propagation direction for the AlN/LiNbO<sub>3</sub>/Si resonator is the material X direction of LiNbO<sub>3</sub> thanks for the fast wave-travelling velocity and the ultralarge  $k_{\text{eff}}^2$ . The wave is also better-guided in the transversal direction compared to the traditional leaky-SH resonator based on LiNbO<sub>3</sub> substrate.

#### 4.6. Frequency Response

Combining the previous analysis toward a high- $f$ , large-  $k_{\text{eff}}^2$ , and spurious-free response utilizing the nonleaky SH wave, a stack with optimized substrate values is achieved:  $5^\circ$  YX-LiNbO<sub>3</sub>,  $h_{\text{LiNbO}_3}/\lambda = 0.25$ , and  $h_{\text{AlN}}/\lambda = 0.2$ . Figure 12a,b plot the FEM-simulated narrow-band responses of the SH wave in the AlN/LiNbO<sub>3</sub>/Si layered stack compared to LiNbO<sub>3</sub>/Si and LiNbO<sub>3</sub> substrate, as well as wide-band response with periodic structure (1.5D model). Intriguingly, the AlN/LiNbO<sub>3</sub>/Si layered structure enables frequency as high as 3 GHz while the IDT pitch is as large as 1  $\mu\text{m}$ , ensuing good power handling. The  $f$  can further scale up if smaller  $\lambda$  is employed. The frequency or  $v_p$  has been increased by 18%, breaking the frequency limits for SAW resonators and filters and applicable to high-frequency bands in LTE-Advancement Pro and 5G NR.

Comparing admittance curves of the SH modes in AlN/ LiNbO<sub>3</sub>/Si, LiNbO<sub>3</sub>/Si, and LiNbO<sub>3</sub> substrate in Figure 12a, it can be noted that the antiresonances for both AlN/LiNbO<sub>3</sub>/Si and LiNbO<sub>3</sub>/Si are very sharp, indicating a very high-quality factor at parallel-resonance ( $Q_p$ ) due to the elimination of bulk leakage (quality factor at series resonance ( $Q_s$ ) is usually dominated by the transducer resistance  $R_s$  and  $Q_p$  dominated by the acoustic propagation loss).



**Figure 12.** FEM-simulated (a) narrow-band response based on AIN/LiNbO<sub>3</sub>/Si ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ,  $h_{\text{AIN}}/\lambda = 0.2$ ) compared to LiNbO<sub>3</sub>/Si ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ) and Si substrate; and (b) wide-band response based on AIN/LiNbO<sub>3</sub>/Si ( $h_{\text{LiNbO}_3}/\lambda = 0.25$ ,  $h_{\text{AIN}}/\lambda = 0.2$ ) for the nonleaky SH resonators with periodic structure (1.5D model).

In addition, the AIN/ LiNbO<sub>3</sub>/Si layered substrate with the optimized parameters shows an extremely clean response in both narrow and wide spectrums. The Rayleigh mode and Lamb modes are suppressed with  $k_{\text{eff}}^2$  of near-zero. By the analysis and careful design, the novel stack provides high performance, the ability of high frequency, and an extremely clean spectrum from 0 to 6 GHz simultaneously.

## 5. Conclusions

In this study, high-frequency nonleaky SH SAW resonators on AIN/LiNbO<sub>3</sub>/Si are demonstrated with thermal stability, large coupling and spurious-free. The high-velocity Si substrate was used to reduce the propagation leakage into substrate, and 15–30° rotation angles from YX-LiNbO<sub>3</sub> were selected to provide the ultralarge  $k_{\text{eff}}^2$ . A careful trade-off analysis is provided on the AIN coating thickness between the enhanced  $v_p$  ( $f$  for given transducer) and the cost of extra  $k_{\text{eff}}^2$ . Furthermore, the out-of-band and near-band spurious modes in the layered SAW structures were analyzed by using FEM simulations and the requirements for the substrate were derived to avoid the presence of spurious modes. Based on this analysis, a new nonleaky SH resonators with optimized substrate design are obtained, demonstrating the ability with a high frequency of 3 GHz at 1 μm IDT pitch, a high  $k_{\text{eff}}^2$  of 14.4% and a spurious-free response throughout 0–6 GHz, showing a great potential for 5G/6G RF communication systems.

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