BAW Resonator with an Optimized SiO₂/Ta₂O₅ Reflector for 5G Applications

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ABSTRACT: In the present work, a lithium niobate (LN) 43°Y cut LN film is transferred onto a substrate with 11 layers of SiO₂/Ta₂O₅ and solidly mounted resonators with a reflector are successfully fabricated with the multilayer structure. The design method and fabrication process are demonstrated. The finite element model and the Mason model are used. Scanning electron microscopy and atomic force microscopy are used to characterize film quality. An optimized design of a Bragg reflector to suppress the leakage of acoustic energy by thickness shear mode is proven to be effective. The influence of the reflector on parasitic modes and filter out-of-band suppression is analyzed. The resonator for 3.5 GHz shows an effective electromechanical coupling coefficient of 17.9%, and the figure of merit is 40.4, which is suitable for band pass filter on the N78 band with high rejection.

1. INTRODUCTION

An acoustic filter is a key component in the miniaturization of an RF front-end system. Filters based on a bulk acoustic wave (BAW)¹⁻⁵ or a surface acoustic wave (SAW)⁶ are widely used in mobile communication terminals due to their compact size and excellent performance. In the 5G era, the demand for wider bandwidth and higher frequency communication has not only resulted in wide prospects to the filter marker but also posed new challenges to the acoustic filter.

The SAW is a finer width-modulated device whose frequency is limited by the photolithographic line width and is typically used at a low frequency. For 5G applications above 3 GHz, thickness-determined frequency BAW devices are a better choice. The film bulk acoustic resonator (FBAR)¹ and solidly mounted resonator (SMR)²,³ are two successful BAW structures that utilize cavities and Bragg reflector (BR) to constrain acoustic waves, respectively. The film thickness of the BAW device is typically at the sub-micrometer level when the frequency is above 3 GHz. FBAR suffers from a fragile structure due to its cavity-type structure when the film is too thin at a higher frequency. For 5G communication above 3 GHz, SMR seems to be the best choice.⁷,¹⁰

The N78 band covers from 3300 to 3800 MHz, which has a relative bandwidth of more than 14%. The bandwidth of the BAW filter is related to the electromechanical coupling coefficient (K_eff²) of piezoelectric material. AlN-based BAW filters are the most successful commercial application, typically having a relative bandwidth of 4.1%⁹ because of poor K_eff² of AlN. Studies aimed at increasing acoustic filter bandwidth can be divided into two categories. One is performed using Sc-doped AlN on the basis of an AlN-based filter.¹⁰⁻¹³ Using AlScN can increase the K_eff² to 15%, but there is still a problem of excessive dielectric loss.¹³ The other is performed using other materials such as lithium niobate (LN), which have extraordinarily large K_eff² at particular orientations or special modes.

SMR based on 43°Y cut LN with a SiO₂/Mo reflector can reach an effective electromechanical coupling coefficient (K_eff²) of 20%¹³ with a Q factor of 92. And a 36°Y cut LN-based FBAR reaches 21.4% at 800 MHz.¹⁴ Despite the poor Q factor or low frequency, the LN-based resonator shows the potential for large bandwidth application. Unlike the thickness expansion (TE) mode resonator mentioned above, X-cut LN-based FBAR using thickness shear (TS) demonstrates K_eff² of up to 39% but suffers from a disadvantage of the strong coupled slow shear wave.¹⁵ The lateral field excited FBAR¹⁶ based on LiTaO₃ has a high Q value at 4.39 GHz, but the K_eff² is

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only 1.2% and is not suitable for wideband filters. In our recent work, the LN-based BAW resonator with a SiO₂/HfO₂ reflector exhibited a $K_{se}$ of 14.6%, but strong parasitic modes exist.

To develop a high-performance resonator for 5G applications, lithium niobate-based resonators with SiO₂/Ta₂O₅ reflectors were designed and fabricated in this work. The design method is introduced, and the fabrication process is shown. The resonator with an optimized reflector is designed to improve the Q value, and the optimized scheme is verified by experiments. The fabricated resonator achieves an effective electromechanical coupling coefficient of 17.9% and a bandpass filter at the N78 band is designed.

2. METHOD

2.1. Design of the Resonator Structure. The basic part of a resonator is a sandwich-like structure of the LN film between two Al electrodes, where acoustic waves are generated. The film thickness in the sandwich structure determines the resonant frequency of the resonator. TE mode is the main mode of a resonator, and the thickness of the LN film can be calculated by

$$d = \nu / 2 f_p$$

where $d$ is the thickness of the LN film, $\nu$ is the phase velocity of the longitudinal wave of LN, and $f_p$ is the antiresonant frequency. Considering the mass load effect of electrodes, the thickness of LN should be thinner. The Mason model18 is established to ensure the resonant frequency is 3.5 GHz by tuning the thickness of Al and LN. The final thicknesses of the top electrode, LN, and bottom electrode were 100, 730, and 100 nm, respectively.

As the film is friable at a frequency above 3 GHz, the SMR structure is adopted to ensure the structural strength of the resonator. SiO₂ and Ta₂O₅ are used as low acoustic impedance material and high acoustic impedance material of Bragg reflectors, respectively. A typical case (SMR 1) with a film thickness of a quarter longitudinal wavelength in each layer of BR is designed. Layers of BR are determined by a transmission spectrum calculated by the finite element method (FEM) with parameters in Table 1. The transmission spectra of BR with different layers (Figure 1a) indicated that BR with 11 layers can reach a transmissivity of -35 dB at 3.5 GHz.

| materials | density (kg/m³) | longitudinal (m/s) | shear (m/s) |
|-----------|-----------------|-------------------|------------|
| SiO₂      | 2200            | 5931              | 3742       |
| Ta₂O₅     | 6850            | 4868              | 2882       |

Table 1. Parameters of BR Materials

Complete resonator structure is shown in Figure 1b. The Al serves as the electrode, and the overlapping position of the top and bottom electrodes forms an Al/LN/Al sandwich-like structure. The BR with SiO₂ and Ta₂O₅ is stacked below the sandwich structure. The glass substrate is connected with the BR by benzocyclobutene (BCB). The resonator has the shape of a regular pentagon and a ground-source-ground (GSG) port of 50 $\Omega$ is used for the probe test.

2.2. Experiment. The fabrication process is shown in Figure 2. First, the 43°Y cut LN wafer is injected with He⁺ under 300 keV to form a defective layer of 980 nm under the injected surface. After preparing a patterned mask by a lithography process, Al is deposited on the surface of LN by magnetron sputtering. Then, SiO₂ and Ta₂O₅ are grown alternately above the surface of Al, forming an 11-layer stacked structure of the Bragg reflector. After spinning of BCB at the surface of SiO₂ under 1000 rpm, a glass substrate is bonded together by the BCB layer. By annealing at 350 °C for 3 h, the LN is separated from the defective layer, and a 980 nm-thick LN film is transferred to the substrate. Then, the peeling surface of LN is etched by RIE for 85 min to thin the LN film to 730 nm. The patterned Al is deposited on the etched surface of the LN film by lithography and magnetron sputtering processes. After deposition of 3 $\mu$m of Al for the pad electrode, the resonator is finally fabricated.

The cross-section morphology is characterized by scanning electron microscopy (SEM). The S parameter of the resonator is tested with a vector network analyzer (VNA) with a GSG probe of MPI. The surface roughness of the LN film is characterized by atomic force microscopy (AFM).

3. RESULTS AND DISCUSSION

Figure 3 shows the simulated impedance curve of the sandwich structure and SMR 1 by the Mason model. The impedance curve of the FBAR structure is clean and with a sharp peak and valley of the main mode. As for the SMR 1 structure, the resonant frequency remains unchanged, but the series impedance increases. The antiresonant frequency and parallel impedance of SMR 1 are significantly smaller than those of the FBAR structure. In addition, several small modes, mode A (Mₐ) and mode B (M₇), appear in the SMR 1 structure with the adoption of the Bragg reflector structure. Since the Mason
model is a one-dimensional model of the longitudinal wave and $M_A$ and $M_B$ can be observed in the simulation result. $M_A$ and $M_B$ are the modes of vibration in the thickness direction caused by the reflector. The frequency of $M_A$ is lower than those of the TE mode and $M_B$ because $M_A$ is caused by the interface between the SiO$_2$ layer and the BCB layer. The lower frequency corresponds to the large wavelength. The frequency intervals between different $M_A$ are uniform, indicating that the three modes of $M_A$ are the same mode of a different order. The generation mechanism of $M_B$ will be discussed later.

The fracture appearances of SMR 1 are shown in Figure 4a. Eleven layers of SiO$_2$ and Ta$_2$O$_5$ are distributed alternately, with clear interfaces. The thickness of SiO$_2$ in SMR 1 is about $419\pm436$ nm, which deviates $-1$ to $3.1\%$ from the designed thickness. And the thickness of Ta$_2$O$_5$ is about $344\pm356$ nm, which deviates about $-1.3$ to $2.3\%$. The thickness of the LN film is $768$ nm, which is $38$ nm thicker than the design value. This deviation is mainly due to the slower etching rates than expected.

Since the rough surface of LN may lead to acoustic scattering and decrease the quality value of the resonator, the roughness of the LN surface is measured by AFM before and after the etching process. As shown in Figure 5a,b, the surface roughness of the peeled LN film is about $7.9$ nm, and the surface etched by RIE has a smaller roughness of $4.2$ nm. The surface roughness of the high $Q$ resonator is preferably less than $1$ nm, which while the etched film roughness is on the order of several nanometers. This indicated that the trimming process can improve the $Q$ value of the device to a certain extent, but to further improve the device performance, it is better to polish the etched surface again.

The $S$ parameter of a resonator is measured by VNA and calibrated before testing. As shown in Figure 5d, the resonant frequency of SMR 1 is $3.453$ GHz, and the antiresonant frequency is $3.72$ GHz. The resonant frequency of the test is $47$ MHz lower than the design, which is mainly caused by the thickness deviation of the LN film. The effective electromechanical coupling coefficient calculated by eq 2 is $17.7\%$.

$$k_{\text{eff}}^2 = \frac{\pi^2}{4} \frac{f_p - f_s}{f_p}$$

where $f_s$ and $f_p$ are the resonant frequency and antiresonant frequency, respectively. The resonator has an impedance ratio of $40.3$ dB. The quality factor of the resonator is calculated with eq 3 and curves of Bode $Q$ are shown in Figure 5f.

$$Q_{\text{bode}} = \frac{\omega \tau |S11|}{1 - |S11|^2}$$

where $\omega$ is the angular frequency and $\tau$ is the group delay of measured $S11$. The conventional design has a maximum $Q_{\text{bode}}$ of $165$ at $3.607$ GHz. The calculated figure of merit (FOM) is $29.3$ for SMR 1.
Typically, the velocity of the shear wave is slower than that of the longitudinal wave, which is about half of the longitudinal wave. As a result, the higher-order mode of the shear wave is resonant together with the longitudinal wave. But the difference in the wave velocity of BR results in noncoincidence between the reflection interval of the shear wave and the longitudinal wave in the 1/4λ design of BR [see Figure 4(c)]. Therefore, only the longitudinal wave is constrained in the design frequency range. The unconstrained shear wave causes leakage of acoustic energy.21

To enhance the shear wave reflection at 3.5 GHz, the thickness of the reflector is adjusted in SMR 2, as shown in Figure 4b. Figure 4d shows the corresponding transmission spectrum of SMR 2. A new reflection region of the shear wave appears at the target frequency, which is relatively consistent with the longitudinal wave. The optimized reflector can ensure that the transmissivity values of both the shear wave and the longitudinal wave are less than −18 and −32 dB at 3.5 GHz, respectively.

As for the optimized SMR 2, the antiresonant frequency is unchanged even at 3.72 GHz. But the resonant frequency is 3.45 GHz, which is 3 MHz lower than that of a nonoptimized resonator. The corresponding \( K_{\text{eff}}^2 \) is 17.9%. It is obvious that the impedance curve at both frequencies becomes sharper, and \( Z_r \) is improved by 7.1 dB. As shown in Figure 5e, the smith chart of an optimized resonator is obviously bigger than that of the traditional one, especially at the antiresonant frequency.

The quality factor of SMR 2 is 225 in Figure 5f, which increases by 60 compared with that of the nonoptimized resonator. By comparing the two curves of quality factor, there is an obvious disturbance between 3.625 and 3.749 GHz in SMR 1, which does not appear in SMR 2, indicating that part of the energy leaks out in the form of a shear wave. The optimized BR can effectively suppress the leakage of acoustic energy by a shear wave. The calculated figure of merit (FOM) is 40.4 for SMR 2. Optimization of the reflector increased the FOM value by 10.1. In addition, the optimized resonator also has a bigger FOM than the LN-based resonator with a reflector of Mo/Ti22 or SiO2/Mo13 for longitudinal waves only.

Thickness change in BR causes only a slight upward shift in the frequency of MA. The slightly increased frequency of MA in SMR 2 also corresponds to a decrease in the total thickness of the reflector. \( M_B \) is more sensitive than \( M_A \). When the structure comes to SMR 2 with optimized BR, both the frequency and strength of \( M_B \) change. Multiple uniformly distributed modes B in SMR 1 turn into one stronger and several weaker modes in SMR 2. It is easy to associate mode B with the interface in the reflector. The change from regular distribution to irregular distribution is consistent with the thickness change of layers in the reflector. \( M_B \) is the resonant mode of longitudinal waves at the reflector interface. The slightly enhanced reflection region in the N79 band contributes to the stronger mode B.

It can be seen from Figure 5d that a mode C (\( M_C \)) exists in SMR with both reflector structures and the resonant frequencies are 2.088 and 2.082 GHz for SMR 1 and SMR 2, respectively. This mode cannot be observed from the simulation results of the Mason model, which is different from mode A and mode B. To further analyze the modes in the resonators, finite element models of two resonators are established. Figure 6 shows the simulated displacement amplitude of mode C in SMR 1 with thickness enlarged. Mode C propagates along the thickness direction and resonates mainly along the horizontal \( v \) direction, which is a TS mode. The shear wave is constrained in the LN film. The displacement distribution of mode C in SMR 2 is very similar to that of SMR 1. Both resonators have a good reflection effect.
The presence of $M_A$, $M_B$, and $M_C$ may cause fluctuation of suppression out of band, especially the enhanced $M_B$ of SMR 2. To evaluate the influence of parasitic mode on the filter, a filter for the N78 band is designed with the Mason model based on the optimized resonator structure. The impedance curve of SMR 2 is fitted with the actual structure by the Mason model. As shown in Figure 7a,b, the fitting result considering losses agrees well with the test result. The extracted contact loss and dielectric loss of LN by the Mason model are 1 and $0.33 \, \Omega$ respectively. The series and parallel resonators of the designed filter have different top electrode thicknesses. The top electrode thickness of series resonators is 100 nm, and the top electrode thickness of parallel resonators is 214 nm. The $S$ parameters and topological structure of the filter are shown in Figure 7c,d. The prototype of a 9-order filter with a ladder-type topology has an insertion loss of 1.81 dB at 3.5 GHz, and the 3-dB bandwidth is 7%. Suppression of the N79 band is $-38$ dB, lower than those of other bands due to enhanced $M_B$. The overall stopband rejection can reach an encouraging $-50$ dB or less with a coefficient of rectangularity of 40 dB/3 dB of 1.38.

4. CONCLUSIONS

In conclusion, a single-crystalline LN film was successfully transferred to a substrate with multilayers of SiO$_2$/Ta$_2$O$_5$. The fabrication process was still feasible on a substrate with up to 11 thin films. LN-based resonators with a Bragg reflector of SiO$_2$/Ta$_2$O$_5$ were successfully fabricated. The optimization of the Bragg reflector could effectively suppress the leakage of shear waves and improve the quality factor. The resonator exhibited a FOM of up to 40.4, having the potential to prepare wide bandwidth filters for the N78 band of 5G communication. But designed reflection intervals should avoid parasitic mode frequency overlap; otherwise, out-of-band suppression will be weakened.

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Figure 6. Displacement amplitude distribution of mode C; (a) horizontal $v$ direction of cross section; (b) horizontal $u$ direction; (c) horizontal $v$ direction; and (d) thickness $w$ direction.

Figure 7. (a) Tested and fitted impedance curves and (b) smith chart of SMR 2. (c) $S_{11}$ and $S_{21}$ of designed filter. (d) Topology of designed filter.
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Notes
The authors declare no competing financial interest.

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