HIGH $k_t^2 \cdot Q$ LAMB-WAVE SCALN-ON-SILICON UHF AND SHF RESONATORS

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ABSTRACT

This paper reports, for the first time, on waveguide-based resonators implemented in scandium-doped aluminum nitride-on-silicon (ScAlN-on-Si) stack to simultaneously benefit from large piezoelectric constants of ScAlN and low acoustic dissipation in single crystal silicon. 1 μ m-thick ScAlN film with Sc content of 7% is reactively sputtered on silicon substrates using ac-powered dual-target S-gun magnetron with Al targets containing embedded pure Sc pellets. A Cl₂/H₂ based low-power plasma etching recipe is developed to pattern resonators with smooth vertical sidewalls. In- and out-of-plane waveguide-based resonator prototypes with large electromechanical coupling coefficient (k_t^2) and high quality-factor (Q) are implemented over 80 MHz – 3.5 GHz demonstrating k_t^2 of 0.7%-2.9% and Q of 2000-6400. Specifically, a high $f_0 \times Q$ of 4.3×10^{12} is measured for a resonator at 3.5 GHz, and a high $k_t^2 \times Q$ of 51 is measured at 108 MHz. The large $k_t^2 \times Q$ of ScAlN-on-Si waveguide-based resonators along with lithographical frequency tailorability demonstrate their potential for realization of highly integrated front-end filters for multi-band 5G systems.

INTRODUCTION

With the exponential growth of wireless users resulted from the emerging internet of things era and the ever-increasing quest for higher data rates, the new generation of wireless systems (i.e. 5G) target integration of multi-band RF transceivers to enhance communication capacity. To enable multi-band transceivers, there is an urgent need for an acoustic resonator technology that simultaneously provides extensive on-chip frequency tailorability while sustaining large k_t^2 and Q . Benefiting from lithographical frequency scalability AlN Lamb-wave resonators are potential candidates for realization of integrated multi-band RF filters [1-3]. However, to materialize such potential Lamb-wave resonators must overcome their shortcomings in major resonator performance metrics, i.e. the coupling coefficient (k_t^2) and quality factor (Q), that are significantly lower compared to thickness-extensional bulk acoustic counterparts (i.e. FBAR and SMR). Various approaches are exploited to improve the k_t^2 of Lamb-wave resonators, including the use of two-dimensional vibration modes that simultaneously benefit from two or three piezoelectric constants for enhanced transduction, or opting for alternative materials, such as lithium niobate (LiNbO₃) with enhanced piezoelectric properties. While two-dimensional vibration modes provide a higher $k_t^2 \times Q$ compared to lateral-extensional counterparts, reaching the performance of FBAR / SMR has remained a formidable challenge. Besides, opting for LiNbO₃ to replace AlN imposes fabrication and integration complexities and results in resonators with significantly larger temperature sensitivity due to the large temperature coefficient of elastic constants. To address the challenge of low k_t^2 in Lamb-wave resonators, a recent wave of research efforts focuses on enhancing the piezoelectric properties of AlN films through introduction of scandium (Sc) doping [4-6]. Experimental studies on the piezoelectric characteristics of Sc-doped AlN (i.e. ScAlN) thin films has shown a 400-500% improvement in the piezoelectric coefficients for a doping concentration of 40% [7]. Such an improvement translates to a k_t^2 of ~30% [6], a value that is 4-5 times larger compared to state-of-art thickness-mode AlN FBARs.

Although successful in improving the k_t^2 , ScAlN Lamb-wave resonators suffer from low Q s that are nearly an order of magnitude lower compared to FBARs at the same frequency. The degradation in Q with Sc doping can be attributed to (a) formation of (100)-crystalline inclusions in (002) oriented ScAlN films [6] and (b) non-ideal etching profile of the films that results in rough and tapered sidewalls [8].

To surpass the limitations with the low Q of ScAlN resonators, this paper presents a new technology that fuses the high k_t^2 of ScAlN films with ultra-low acoustic dissipation of single crystal silicon to realize Lamb-wave resonators with large $k_t^2 \times Q$. ScAlN film with reduced density of inclusions is sputtered on silicon substrate and etched through a low-power RIE process that yields smooth sidewalls. Dispersion engineering of ScAlN-on-Si waveguides are used to implement resonators with large $k_t^2 \times Q$ and lithographical frequency scalability over UHF and SHF.

RESONATOR DESIGN

Resonators with high k_t^2 are designed using acoustic engineering of ScAlN-on-Si waveguides. The dispersion characteristic of Lamb waves is used to realize energy localization of extensional waves thorough cascading ScAlN-on-Si waveguides with different lateral dimensions. In this approach the dimensions of constituent waveguides are chosen to enable acoustic coupling of extensional bulk acoustic waves in the central electroded region with evanescent waves in the flanks. Figure 1 demonstrates the SEM image of a waveguide-based resonator and the dispersion characteristic of the constituent waveguides that are used for energy trapping of the 5th width-extensional (WE₅) mode with a high k_t^2 .

Figure 1: SEM image of a waveguide-based resonator operating in the 5th width-extensional mode. The inset shows dispersion curves of the corresponding Lamb waves that forms the mode, for constituent waveguides (i.e. regions I-III). The corresponding solutions at the resonance frequency are highlighted by stars.

Figure 2: (a) Waveguide-based resonator concept: cascaded waveguides with varying widths. (b) COMSOL mode-shape of the device. (c) Normalized energy across the central axis of the device showing “piston”-shaped mode of vibration.

The corresponding solutions in constituent waveguides that contribute to form the resonance mode are highlighted through stars. Figure 2 demonstrates the COMSOL-simulated mode shape for the resulting WE_5 mode. Opting for proper length of the waveguides to satisfy displacement and strain continuity at transitions, the bulk acoustic wave ($k_x = 0$) in the central region (i.e. region I) can be coupled to evanescent waves in the flanks (i.e. region III), through Lamb waves with finite wavelength ($k_x \neq 0$) in region II. Figure 2(c) demonstrates the normalized acoustic energy across the central axis of the waveguide-based resonator in Figure 1. The proper acoustic engineering has resulted in a uniform energy distribution over the central / electrode region, which translates to a large kt^2 . Furthermore, the exponentially decaying acoustic energy in flanks is evident, which results in efficient energy trapping of the WE_5 mode with a high Q . In this paper the dispersion-based acoustic engineering is used for realization of high kt^2 waveguide-based resonators operating in width-extensional harmonics as well as fundamental thickness-extensional modes over UHF and SHF regimes.

FABRICATION PROCESS

A stack of $1\mu\text{m}$ ScAlN film with Sc content of 7%, sandwiched between 50-100nm molybdenum (Mo) layers, is reactively sputtered on single crystal silicon substrate using ac-powered dual-target S-gun magnetron with Al targets containing embedded pure Sc pellets [9]. This technique enables the growth of ScAlN film with strong (002) preferred orientation (FWHM = 1.89°) and low stress of -189MPa. Proper optimization of processing condition enables reduction of the density of (100) conical intrusions in the film. Top Mo layer is patterned to form input and output transducers in the active region of the waveguide-based resonator. This is followed by dry-etching of ScAlN film. Unlike AlN, ScAlN films are highly resistant to BCl_3 -based RIE recipes, resulting in very low etch rates and poor selectivity to photoresist or silicon dioxide mask layers. Furthermore, the Sc-based non-volatile byproducts of the etching process remains / accumulates during the etching process [8], which results in undesirable nano-masking of subsequent etching of bottom Mo in trenches as well as DRIE of silicon and yields waveguides with rough sidewalls and consequently low Q . To address the etching challenges of ScAlN while sustaining a reasonably low RIE/ICP power and high etching selectivity, a Cl_2/H_2 based RIE recipe is developed to realize comparable etch rates to AlN thin films. Besides improving the etch rate, the developed recipe physically removes the Sc-based byproducts

Figure 3: Fabrication process flow for the resonators with different Si thickness: (a) MO/ScAlN/Mo/Si stack. (b) Top Mo Patterning (c) Timed etching of ScAlN/Mo/Si selectively to get the desired silicon-substrate thicknesses. (d) Backside DRIE of silicon to release the devices. Backside etch timed to release the device with desired

Table 1: ScAlN RIE process parameters.

Parameter	Values
Cl_2 flow rate (sccm)	60
H_2 flow rate (sccm)	40
He flow rate (sccm)	10
RF Bias (W)	100
ICP Bias (W)	300

resulting in smooth surface after etching ScAlN film. In the next step, silicon layer is etched through Bosch DRIE of silicon substrate from top and bottom to form the released acoustic cavity with proper lateral geometry. Figure 3 summarizes the fabrication process flow. Samples with different silicon trench depths are prepared and released through proper timing of the backside DRIE to facilitate implementation of waveguides with different silicon thicknesses

Figure 4: (left) SEM images of ScAlN-on-Si waveguide-based resonator operating in the fundamental width-extensional mode. (right) the cross-sectional SEM of the resonator detailing the ScAlN sidewall, after RIE in Cl_2 / H_2 , and Si, after Bosch DRIE. A hard mask of SiO_2 is used for etching the resonator stack.

Figure 5: SEM images of (a) 3rd, (b) 5th, and (c) 7th width-extensional ScAlN-on-Si resonators. Waveguides are acoustically engineered through coupling evanescent and propagating waves to enable efficient energy trapping of the targeted Lamb-wave.

(Design I-III). This enables experimental evaluation of the effect of silicon on resonator Q and k_t^2 . Table 1 summarizes the ScAlN RIE process details, highlighting the gas composition and low bias power. Figure 4 (a) demonstrate the SEM image of the ScAlN-on-Si waveguide-based resonator operating in fundamental width-extensional mode. Figure 4 (b) demonstrate the cross-sectional SEM of an unreleased waveguide after trench etching. The smooth and tapered sidewall profile of the ScAlN as well as an etch-resistant (100) conical intrusion are evident. The tapered profile of ScAlN sidewall is due to the high pressure of constituent gases that is used to facilitate removal of Sc-based non-volatile compounds. Figure 5 shows the SEM images of 3rd, 5th and 7th width-extensional resonators implemented in ScAlN-on-Si (0-6 μ m silicon thickness). Interdigitated electrodes are patterned lithographically within the active region (i.e. central waveguide) of the resonators to facilitate excitation of width/thickness-extensional modes with high k_t^2 .

CHARACTERIZATION

Two-port ScAlN-on-Si Lamb-wave resonators with various silicon thicknesses are implemented and characterized to facilitate

Figure 6: Measured frequency response of ScAlN-on-Si waveguide-based resonators with different silicon thicknesses. Increasing the silicon thickness from 0 to ~6 μ m improves the Q with ~1-order of magnitude, resulting in a high $k_t^2 \times Q$ of 51.

Figure 7: Measured frequency response of the high-order ScAlN-on-Si resonators shown in Figure 5, with frequencies over 250 MHz to 3.5 GHz. The inset shows the COMSOL-simulated mode shapes.

comparison of the k_t^2 and Q and experimental quantification of the enhancing effect of silicon substrate on $k_t^2 \times Q$. Figure 6 demonstrate the measured frequency response of resonators with different silicon thicknesses (i.e. 0-6 μ m). While the increase in silicon thickness reduces the k_t^2 , the Q of the resonator is significantly enhanced thanks to the ultra-low acoustic dissipation of single crystal silicon, resulting in a high $k_t^2 \times Q$ of 51 measured at 108 MHz. The presence of multiple closely placed peaks with comparable Q can be attributed to (100) conical intrusions as well as tapered sidewalls of the ScAlN film resulted from RIE process. Figure 7 shows the short-span frequency responses for higher-order extensional and thickness-mode resonators shown in Figure 5. High

Table 2: The summary of measured performance metrics of fundamental-mode and high-order Lamb-wave ScAlN-on-Si resonators shown in Figure 1 and Figure 3. A record high $f_0 \times Q$ of 4.3×10^{12} is measured at 3.5 GHz, which is the highest ever-reported value for any ScAlN-based resonator.

Mode Shape	Q	f	$f \times Q$
3 rd WE Mode	1780	251.3MHz	4.4×10^{11}
5 th WE Mode	2140	259.1MHz	5.5×10^{11}
7 th WE Mode	2856	671.2MHz	1.9×10^{12}
Thickness Extensional	1240	3.51GHz	4.3×10^{12}
Fundamental Mode	6386	106MHz	6.7×10^{11}

Figure 8: Temperature characteristic of frequency for pure ScAlN Lamb-wave resonator, compared to AlN counterpart.

Q s over 1300-2900 are measured for waveguide-based ScAlN-on-Si resonators operating over 250MHz-3.5GHz in width/thickness-extensional modes. Such high Q s is a result of ultra-low acoustic dissipation of single crystal silicon as well as efficient acoustic energy localization that suppresses energy leakage out of the resonator active region.

Table 2 summarizes the performance metrics of the resonators in Figure 4 and 5. A record high $f_0 \times Q$ of 4.3×10^{12} is measured for an ScAlN-on-Si resonator at 3.5 GHz, which is the highest ever-reported value for any ScAlN-based resonator. Moreover, similar high $f_0 \times Q$ values are measured for resonators operating at 100-700MHz and summarized in Table 2.

Finally, Figure 8 demonstrates the temperature characteristic of the frequency for ScAlN waveguide-based resonator operating in fundamental width-extensional mode. A similar design is used to implement an AlN resonator; hence, facilitating the evaluation of the effect of Sc doping on linear temperature coefficient of frequency (TCF_1). TCF_1 of $-33.4 \frac{\text{ppm}}{^\circ\text{C}}$ and $-25.3 \frac{\text{ppm}}{^\circ\text{C}}$ are measured for AlN and ScAlN resonators, respectively. The close TCF_1 values for AlN and ScAlN facilitates integration of ScAlN-based resonators into frequency control applications through exploiting similar compensation techniques that are well developed for AlN counterparts.

CONCLUSION

This paper presents high- Q ScAlN-on-Si waveguide-based resonators with lithographically defined frequencies over UHF and SHF regimes. The combination of high- k_t^2 of Sc-doped AlN film with ultra-low acoustic dissipation in single crystal silicon results in the enhancement of resonator $k_t^2 \times Q$. Acoustic engineering of the waveguides based on dispersion characteristics of Lamb-waves is used to efficiently trap the acoustic energy with a uniform energy distribution in active region. New recipes for deposition and etching of ScAlN are developed to yield films with low distribution of (100) intrusions and smooth sidewall etching profile. Waveguide-based resonator prototypes operating in fundamental and harmonics of width- and thickness-extensional modes are implemented over 80 MHz – 3.5 GHz demonstrating k_t^2 of 0.7%-2.9% and Q of 2000-6400. Specifically, a high $f_0 \times Q$ of 4.3×10^{12} is measured for a resonator at 3.5 GHz, and a high $k_t^2 \times Q$ of 51 is measured at 108

MHz. The large $k_t^2 \times Q$ of ScAlN-on-Si waveguide-based resonators along with lithographical frequency tailorability demonstrate their potential for realization of highly integrated front-end filters for multi-band 5G systems.

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