Towards Unparallelled CMOS-compatible Air-coupled pMUT Performance with 30% Sc-doped AlN through an Analysis of Residual Stress Effects

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Abstract— **Aluminum Nitride (AlN) offers a CMOS-compatible, stable, and lead-free solution for piezoelectric micromachined ultrasonic transducers (pMUTs), if not for its limited $e_{31,f}$ piezoelectric coefficient. Even though increasing scandium (Sc) doping content in ScAlN is known to enhance the electromechanical coupling factor (K_t^2) and overall acoustic performance, the outcome is highly dependent on the stress of the ScAlN film especially for air-coupled pMUTs. This study aims to compare pMUT performance (in terms of K_t^2) due to increasing Sc content from 20% to 30% in relation to stress and considering its effects on frequency and static deformation of the membrane. Results show that 30% Sc devices achieved an average K_t^2 >6% at -50 MPa, on par with PZT-based pMUTs. Compared to 20% Sc, the 30% Sc-doped pMUTs demonstrated a 50% increase in transmit pressure sensitivity and overall 6 dB increase in two-way sensitivity.**

Keywords— ***ScAlN, pMUT, residual stress, electromechanical coupling factor***

I. INTRODUCTION

Scandium Aluminum Nitride (ScAlN) has emerged as a material of significant interest in the field of piezoelectric Micro-Electro-Mechanical Systems (MEMS) devices. Its unique properties and enhanced performance characteristics position it as an increasingly attractive option for various applications. Compared to conventional Aluminum Nitride (AlN), ScAlN's superior piezoelectric properties enable more efficient energy conversion between electrical and mechanical domains, particularly in piezoelectric micromachined ultrasonic transducer (pMUT) applications [1]. In contrast to Lead Zirconate Titanate (PZT), ScAlN's inherent piezoelectricity and absence of ferroelectric hysteresis make it an optimal choice for resonant micro diaphragm sensor applications, ensuring more stable and predictable performance [2]. Furthermore, ScAlN's compatibility with standard Complementary Metal Oxide Semiconductor (CMOS) processes and high temperature stability render it particularly advantageous for integrated circuit (IC) integration [3], facilitating the development of compact, portable applications.

The enhancement of piezoelectric properties through increased Sc doping concentration has been well-established as an effective method for improving both transmit (Tx) and receive (Rx) performance in pMUTs. Liu et al. demonstrated a Finite Element Method (FEM) Multiphysics modelling approach to predict the performance of Sc-doped AlN pMUTs [4]. Their calculations revealed a monotonic increase in electromechanical coupling coefficients from 0.5% to 3.7% as doping concentrations increased from 0% to 40%, corresponding to approximately 3.5-fold improvement in Tx sensitivity and 2-fold enhancement in Rx sensitivity. In a practical implementation, Choong et al. developed a hybrid rangefinder utilizing ScAlN pMUTs as receivers [5]. This research showcased a 20% Sc-doped concave pMUT with a Rx sensitivity of 22 mV/Pa, representing a 2-fold increase compared to a 15% Sc-doped convex pMUT.

Despite these promising advancements, fabrication-induced residual stress remains a critical and often underestimated factor that affects pMUT performance. This unpredictable phenomenon can significantly impact device characteristics, potentially offsetting the benefits gained from increased Sc doping. Prior study [6] has shown that residual stress can cause substantial (e.g. ±80 kHz) shifts in resonant frequency. More concerning is its impact on K_t^2, which can be drastically reduced from an optimal value of 3% to as low as 0.5%, severely compromising device efficiency.

Given the critical interplay between Sc doping and residual stress, there is an urgent need for comprehensive research exploring the relationship and its impact on device performance. This study addresses this gap by investigating the effects of increasing Sc doping from 20% to 30% on pMUT performance, with a particular focus on K_t^2. Our work considers the complex interactions between Sc doping, residual stress, resonant frequency, and static membrane deformation. Experimental validation includes measurements of Tx displacement and pressure sensitivity for transmission capability, and Rx voltage sensitivity for receive capability. This multifaceted approach provides a thorough insight into optimizing ScAlN pMUT performance through control of Sc doping and stress management.

II. DESIGN AND SIMULATION

A. Design of pMUT

To facilitate a direct comparison, identical pMUT designs were fabricated using our Lab-in-Fab (LiF) 8-inch wafer-scale platform [6], with the key distinction being the Sc concentration in the ScAlN film (20% vs 30%, deposited using the same tool). An optical image and cross-sectional schematic of the pMUT used in this study are presented in

Fig. 1. (a) and Fig. 1. (b). A 480 µm-wide diameter cavity and 70% piezoelectric stack diameter covering ratio are designed to target 150 kHz resonant frequency while optimizing electrical to mechanical energy conversion efficiency. The pMUT architecture comprises a circular 3 µm-thick epi-Si membrane that supports a 1 µm-thick $Sc_xAl_{1-x}N$ (x= 0.2 or 0.3) layer with top and bottom metal electrodes (0.2 µm-thick Mo).

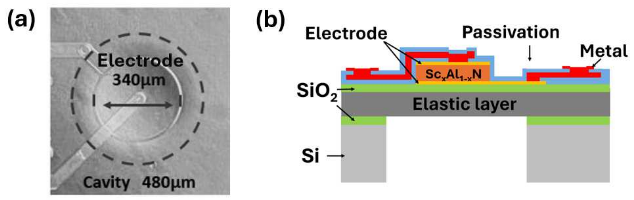

Fig. 1. (a) Top view and (b) Cross-section view of $Sc_xAl_{1-x}N$ pMUT.

B. *Experiment setup*

Our comprehensive experimental approach encompassed both wafer-level and single-chip characterization to elucidate the impact of increasing Sc content from 20% to 30% on pMUT performance as illustrated in Fig. 2. Wafer-level analysis included residual stress mapping of piezoelectric stack before wafer release using an FSM 128 C2C system and extraction of resonant frequency and K_t^2 using a Keysight E4990A Impedance analyzer with a SUSS PA-200 semiautomatic probe station under atmosphere. These measurements enabled correlation between initial stress, pMUT resonant frequency, and K_t^2. Single-chip characterization employed an optical profiler (Sensofar Metrology S wide) for static deformation measurement, a Laser Doppler Vibrometer (Polytec MSA-500) for mechanical characterization, and a microphone (Avisoft-Bioacoustics CM16/CMPA40-5V) for acoustic characterization in both Tx and Rx modes. This multi-faceted approach provided comprehensive insights into the relationship between Sc doping, stress variations, and pMUT performance, which are helpful for informing process optimization strategies.

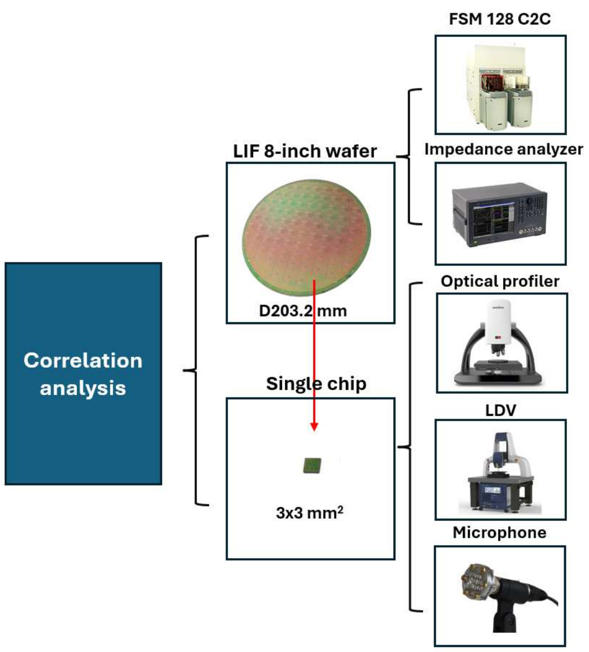

Fig. 2. Test scheme for wafer level and chip level device with the corresponding test setup.

III. RESULTS AND DISCUSSION

Results from full-wafer impedance analysis of 45 devices per wafer, coupled with wafer-level film stress measurements, revealed significant insights into the effects of Sc doping and residual stress on pMUT performance. The frequency response of 30% Sc and 20% Sc pMUTs exhibited distinct behaviors under varying residual stress conditions as shown in Fig. 3. For 30% Sc pMUTs, as stress changed from -80 MPa to +150 MPa, the resonant frequency initially decreases from 190 kHz to 126 kHz, then increases to 208 kHz. In contrast, 20% Sc pMUTs showed a monotonic increase in resonant frequency from 150 kHz to 242 kHz as stress shifted from -125 MPa to +125 MPa. This difference indicates that the 30% Sc doping piezo stack, with lower stiffness, is more susceptible to residual stress.

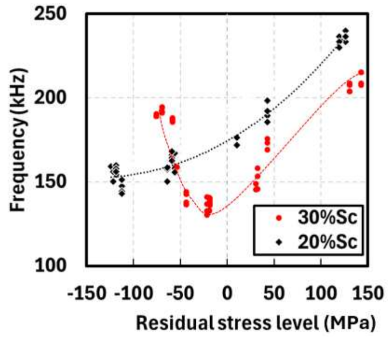

Fig. 3. Wafer level results of frequency versus residual stress.

The K_t^2 also demonstrated a correlated trend with residual stress for both 30% Sc and 20% Sc pMUTs in Fig. 4. Generally, higher tensile stress leading to higher frequencies resulted in lower K_t^2 values. For 20% Sc pMUTs, K_t^2 monotonically decreases from 4.8% to 0.1% as the stress changes from compressive to tensile. The 30% Sc pMUTs, however, exhibited a maximum K_t^2 of 8% at approximately -50 MPa, comparable to PZT pMUTs in prior studies. Notably, within the same stress range (-50 MPa to +50 MPa), 30% Sc pMUTs consistently demonstrated higher K_t^2 values compared to 20% Sc pMUTs, attributed to enhanced piezoelectric constants and the softening effect of lower stiffness. These findings suggest highlight the potential of 30% Sc pMUTs for superior efficiency in both Tx and Rx acoustic performance within this stress range.

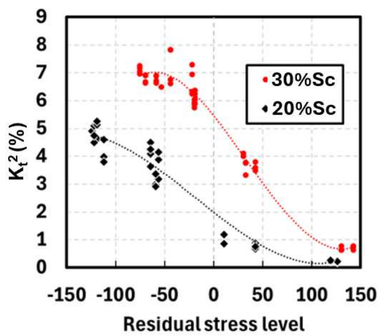

Fig. 4. Wafer level results of K_t^2 versus residual stress.

Following wafer-level analysis, chip-level tests were conducted on selected pMUT samples with equivalent Sc stack stress conditions (-50 MPa) for both 30% and 20% Sc compositions. The chips were mounted on PCBs with bonding wires and SMA ports to ensure reliable electrical connectivity. Electrical impedance spectroscopy with magnitude and phase are depicted in Fig. 5, revealing that the

30% Sc device exhibited a slightly lower resonant frequency compared to its 20% Sc counterpart, but demonstrated a notable 2.4-fold higher K_t^2.

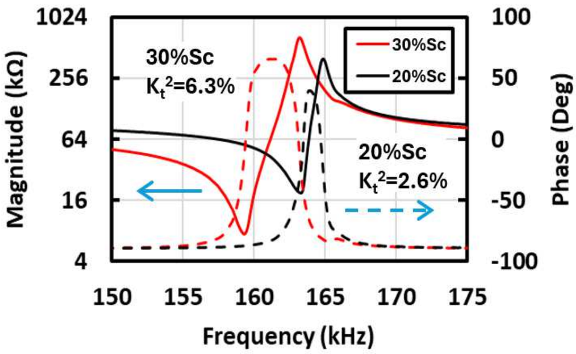

Fig. 5. The impedance spectrum of magnitude and phase for 30% Sc and 20% Sc devices under same initial stress status.

Static deformation measurements in Fig. 6 showed nearly flat profiles for both samples in their initial states. However, the 30% Sc pMUT displayed a slightly larger concave deformation (0.2 μm) compared to the 20% Sc device, consistent with its lower Young's modulus. This minor difference in initial deformation aligns well with the observed trends in the impedance spectra, further validating the relationship between mechanical properties and electrical performance. It's worth noting that while the Sc stack stress is the primary factor influencing the overall stack behaviours, the additional 0.7 μm passivation SiO_2 layer also contributes to the final static deformation to some extent.

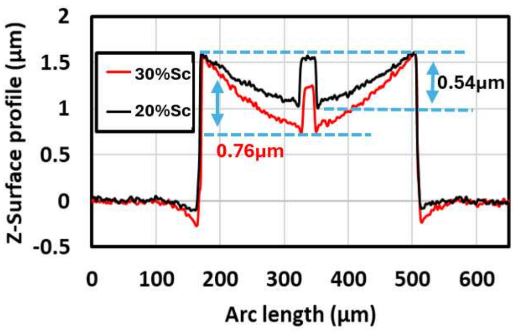

Fig. 6. The optical profiles for 30% Sc and 20% Sc devices.

Dynamic displacement sensitivity was measured using LDV with a 1 Vpp 60-cycle sine small signal drive (Fig. 7). The superior performance of the 30% Sc device is evident from comparing the center displacement sensitivities: 2314 nm/V for 30% Sc, 1.64 times higher than that of the 20% Sc pMUT at resonance (1.5-2.0 times higher under off-resonance).

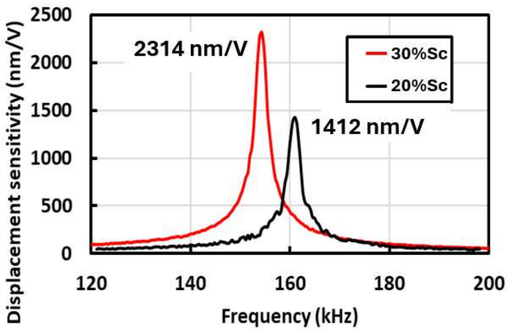

Fig. 7. Tx displacement sensitivity for 30% Sc and 20% Sc devices.

Acoustic performance characterization further demonstrated the superiority of 30% Sc pMUTs over their 20% Sc counterparts. Tx pressure sensitivity measurements, conducted with a condenser microphone placed 10 cm above the pMUT surface following the same driving condition set as the LDV tests, reveals that the 30% Sc pMUT has a pressure sensitivity of 0.13 Pa/V (Fig. 8). This is 1.55 times higher than that of the 20% Sc pMUT, thus having a similar gain factor as observed in the LDV displacement sensitivity tests.

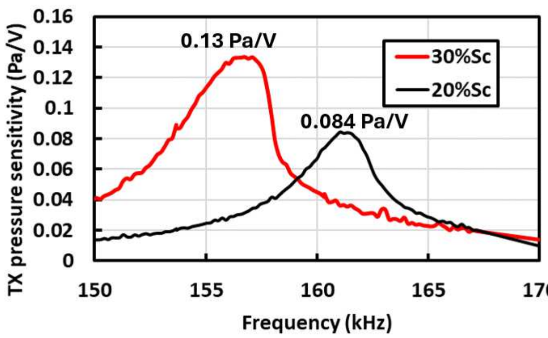

Fig. 8. Tx acoustic pressure sensitivity for 30% Sc and 20% Sc devices.

Rx voltage sensitivity was evaluated using a pitch-catch configuration with one characterized transmitter on one side and a receiver pMUT (either 30% Sc or 20% Sc) on the other side separated by a distance of 10 cm. Under steady state oscillations, induced by a 400-cycle, 20 Vpp signal applied to the transmitter, the 30% Sc pMUT exhibited a voltage sensitivity of 81 mV/Pa. This result was 1.35 times higher than the sensitivity of the 20% Sc pMUT, further confirming the enhanced performance of the higher Sc content devices in both Tx and Rx modes.

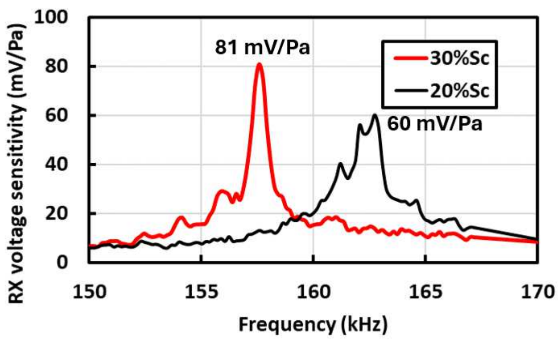

Fig. 9. Rx voltage sensitivity for 30% Sc and 20% Sc.

IV. CONCLUSION

In conclusion, this comprehensive study on the effects of Sc doping and residual stress on ScAlN pMUT performance has yielded significant insights. Our findings demonstrate that increasing Sc content from 20% to 30% in ScAlN films enhances device performance overall, particularly within the -50 MPa to +50 MPa stress range. The 30% Sc pMUTs exhibited superior K_t^2, with a mean value >6% at approximately -50 MPa, rivaling PZT-based devices. This improvement translated to markedly better acoustic performance, with the 30% Sc pMUTs showing 1.64 times higher displacement sensitivity, 1.55 times higher Tx pressure sensitivity, and 1.35 times higher Rx voltage sensitivity compared to their 20% Sc counterparts.

ACKNOWLEDGMENT

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