Impact of Asymmetric Piezoelectricity of 100 nm $Al_{0.7}Sc_{0.3}N$ Thin Film on Ferroelectrically Switchable Multi-Layer Bulk Acoustic Wave Resonators

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***Summary*— In this paper, we investigate the impact of asymmetric piezoelectricity of the 100nm $Al_{0.7}Sc_{0.3}N$ film on the mode-switchable film bulk acoustic resonator (FBAR), which composes of two stacked ferroelectrically switchable $Al_{0.7}Sc_{0.3}N$ layers. A high overtone bulk acoustic wave mode test structure is designed and fabricated to extract the piezoelectric properties of the 100nm $Al_{0.7}Sc_{0.3}N$ film at positive and negative polarization states. It is found that the film exhibits different electromechanical coupling constant (K_t^2) of 11.8% and 7.9% at different polarities. The theoretical model built upon the extracted material parameters suggests that two resonant frequencies at around 10GHz and 18.5GHz can be obtained in a FBAR with stacked 100nm $Al_{0.7}Sc_{0.3}N$ dual films in between 50nm Mo electrodes. The effective coupling coefficient (K_{eff}^2) can be tuned between 19.7% and 12.7% at the 10GHz mode by aligning both $Al_{0.7}Sc_{0.3}N$ films at positive or negative polarization, respectively. While switching to make the two films at opposite polarities will boost the frequency to be 18.5GHz with K_{eff}^2 of 18%.**

Keywords— $Al_{0.7}Sc_{0.3}N$; ferroelectric; switchable; BAW resonator

I. INTRODUCTION

The ferroelectric switchable acoustic resonator is a promising solution to reduce the number of filters needed in current mobile devices [1]. Recently, AlScN with excellent CMOS compatibility has been examined to obtain a higher K_t^2 with an increasing scandium doping concentration [2], and ferroelectricity in ultra-thin thickness [3-5]. All these merits of ferroelectric AlScN indicate its potential for achieving switchable bulk acoustic wave (BAW) resonators and filters with a high resonant frequency beyond sub-6GHz band and a wide bandwidth. However, the piezoelectricity of the ferroelectric AlScN thin films around 100nm with different polarization states has not been experimentally characterized, and the impact of the asymmetric piezoelectricity of the ferroelectric film under different polarities on the switchable multi-layer ferroelectric FBAR has not been investigated yet. In this paper, the asymmetric piezoelectricity of 100 nm AlScN film is extracted and its impact on switchable FBAR is studied.

II. METHODS/RESULTS

Fig. 1(a)-(c) show the schematic of a switchable multi-layer ferroelectric FBAR in three operation modes with ferroelectric films under different polarization configurations for simulation. The polarization of the ferroelectric layer can be switched by the applied electric field [Fig. 1(d)]. The HBARs are fabricated

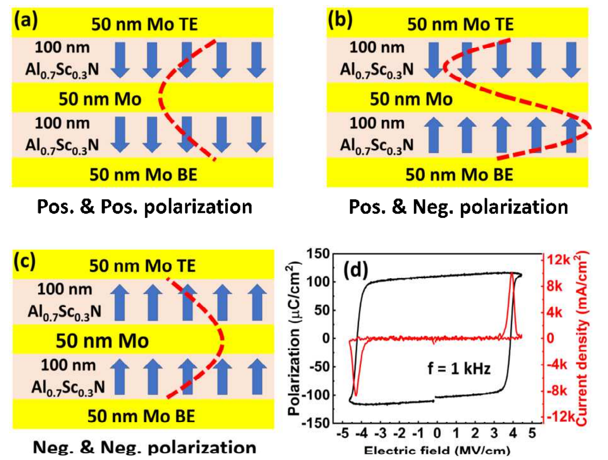

Fig. 1. (a)-(c) The schematic of a switchable multi-layer ferroelectric FBAR in three modes under different polarization states. The positive polarization state refers to the condition of applying a positive pulse with a pulse amplitude larger than the coercive field (E_c) onto the top electrode, while the negative polarization state corresponds to the condition of applying a negative pulse that enables to flip the polarization direction oppositely. (d) The typical *P-E* & transient *J-E* behavior of the 100 nm $Al_{0.7}Sc_{0.3}N$-based MFM device.

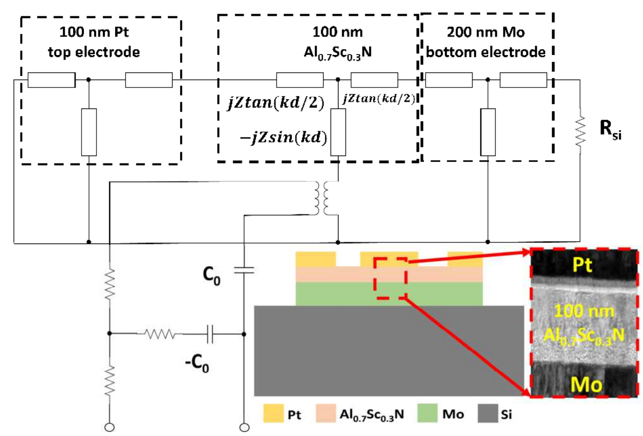

Fig. 2. Cross-sectional schematic and TEM image of the HBAR, in which the 100 nm ferroelectric $Al_{0.7}Sc_{0.3}N$ is deposited by pulse laser deposition (PLD) and sandwiched between a 200 nm Molybdenum layer and a 100 nm platinum layer, and its corresponding equivalent circuit for extracting K_t^2 *via* Mason model.

to extract the piezoelectric parameters of the 100nm ferroelectric $Al_{0.7}Sc_{0.3}N$ film under different polarities. Fig. 2 exhibits the cross-sectional schematic and TEM image of the

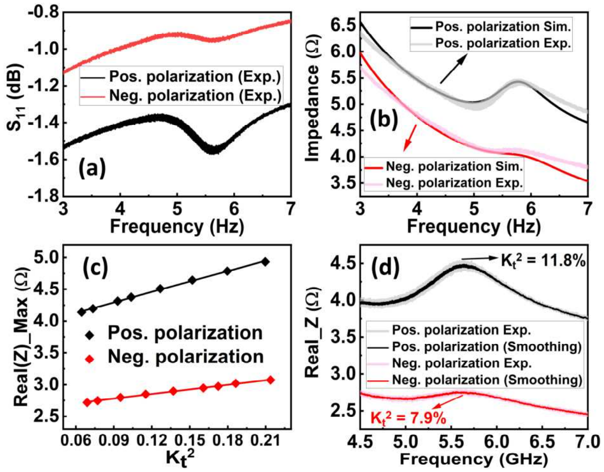

Fig. 3. (a) Measurement result of S_{11} *vs*. frequency of the 100 nm $Al_{0.7}Sc_{0.3}N$ under different polarization directions. (b) Measured and simulated impedance vs. frequency of the 100 nm $Al_{0.7}Sc_{0.3}N$ under different polarization directions. (c) Relationship between maximum of the impedance (real part) and K_t^2 of the 100 nm $Al_{0.7}Sc_{0.3}N$ under different polarization directions. (d) Measured and smoothed real part of the impedance vs. frequency of the 100 nm $Al_{0.7}Sc_{0.3}N$ under different polarization directions.

fabricated HBAR, and its corresponding equivalent circuit. The switchable multi-layer ferroelectric AlScN-based FBAR with different polarization states are then theoretically examined with the extracted material parameters.

III. DISCUSSION/INTERPRETATION

Fig. 3(a) shows the return loss (S_{11}) of the same resonator under different polarization states. Fig. 3(b) shows the measured and simulated impendence, agreeing with each other for both positive polarization and negative polarization states. In the modelling of the lossy HBAR, there would exhibit a proportional relationship between K_t^2 ($K_t^2=e_{33}^2/(c_{33}\times\varepsilon)$) of the material and the maximum of the real part of impedance [Fig. 3(c)] [6]. By mapping the experiments to the simulated curves shown in Fig. 3(c), the K_t^2 is extracted to be 11.8% and 7.9% under positive/negative polarization, respectively [Fig. 3(d)]. To investigate the impact of this asymmetric piezoelectric constant on the switchable resonator, an overtone FBAR device composing of two sub-AlScN layers is simulated (Fig. 4). Switchable resonant frequencies of ~10GHz and ~18.5GHz are achieved by switching the polarization states of the ferroelectric layers. Owing to the asymmetric piezoelectricity with different polarization states, the K_{eff}^2 are extracted to be 19.7% and 12.7% for two ferroelectric layers that are both positively/negatively polarized, respectively [Fig. 4(a)]. In the condition of the two ferroelectric layers being symmetrically/asymmetrically oppositely polarized, the K_{eff}^2 are extracted to be 21.9% and 18%, respectively [Fig. 4(b)]. Additionally, the K_{eff}^2 can be tuned within a wide range by modifying the piezoelectricity of the negative polarity, e.g. partially switching [Fig. 4(c)].

IV. CONCLUSIONS

In this work, the influence of the asymmetric piezoelectricity of the ferroelectric 100nm $Al_{0.7}Sc_{0.3}N$ film on switchable dual-layer FBARs is studied. The asymmetric K_t^2 of 100nm

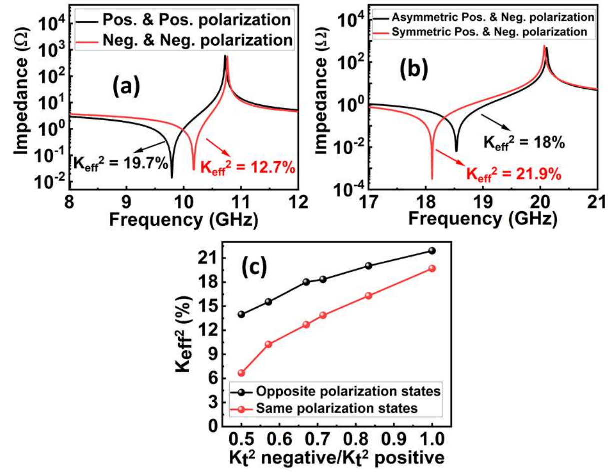

Fig. 4. Simulated impedance response to the frequency of the multi-layer ferroelectric FBAR under different polarization states, where the thickness of the metal electrodes and each $Al_{0.7}Sc_{0.3}N$ layer is 50 nm and 100 nm, respectively. (a) Both ferroelectric layers are positively/negatively polarized [refers to Fig. 1(a), (c)]. (b) Ferroelectric layers have opposite polarization directions to each other [refers to Fig. 1(b). Symmetric opposite polarization corresponds to the assumption that the piezoelectric parameters are the same under positive and negative polarization states, while asymmetric opposite polarization takes the asymmetric piezoelectricity under different polarizations states into consideration. (c) Simulation of K_{eff}^2 considering the change of K_t^2 of negative polarization state compared with positive polarization state, showing that the K_{eff}^2 is tunable by modifying the characteristics of the negative polarization state. In the simulation, the material parameters of positive polarization are fixed, and the same polarization state refers to that both two layers are negatively polarized.

$Al_{0.7}Sc_{0.3}N$ is extracted to be 11.8% and 7.9% under different polarities, respectively. Additionally, both the resonant frequency and K_{eff}^2 of the dual-layer FBARs can be efficiently tuned by controlling the polarities of the ferroelectric film.

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REFERENCES

[1] S. Gevorgian, A. K. Tagantsev, and A. Vorobiev, "Tuneable film bulk acoustic wave resonators," London: Springer, 2013.

[2] G. Wingqvist, F. Tasnadi, A. Zukauskaite, J. Birch, H. Arwin, and L. Hultman, "Increased electromechanical coupling in w-$Sc_xAl_{1-x}N$," *Appl. Phys. Lett.*, vol. 97, pp.112902, 2010.

[3] S. Fichtner, N. Wolff, F. Lofink, L. Kienle, and Wagner, B., "AlScN: A III-V semiconductor based ferroelectric," *J. Appl. Phys.*, vol. 125, pp.114103, 2019.

[4] C. Liu, Q. Wang, W. Yang, T. Cao, L. Chen, M. Li, F. Liu, D. K. Loke, J. Kang, and Y. Zhu, "Multiscale modeling of $Al_{0.7}Sc_{0.3}N$-based FeRAM: the steep switching, leakage and selector-free array," In *2021 IEEE International Electron Devices Meeting (IEDM)*, pp. 8-1, 2021

[5] L. Chen, C. Liu, M. Li, W. Song, W. Wang, Z. Chen, S. Samanta, H. K. Lee, and Y. Zhu, "Bipolar and unipolar cycling behavior in ferroelectric scandium-doped aluminum nitride," In *2022 IEEE International Symposium on Applications of Ferroelectrics (ISAF)*, pp. 1-3, 2022

[6] C. Zhou, W. Pang, Q. Li, H. Yu, X. Hu, and H. Zhang, "Extracting the electromechanical coupling constant of piezoelectric thin film by the high-tone bulk acoustic resonator technique," *IEEE Trans. Sonics Ultrason.*, vol. 59, pp.958-962, 2012.