Impact of In-Plane Residual Stress on The Performance of The Film Bulk Acoustic Resonators

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***Abstract*— This paper presents the effect of in-plane residual stress on the design parameters such as resonance frequency and coupling coefficient of the Film Bulk Acoustic Resonator (FBAR) in accordance with the enhanced experimental buckling observed in the FBAR. The deformation in the film is due to the asymmetry of unequal top and bottom electrode thickness. The simulation models the individual impact that the residual stress has on the geometric and material properties of the thin piezoelectric film. The sensitivities of the individual impact provide design considerations for FBAR. The stack that has an equal thickness of the top and bottom electrodes provides less deformation and a predictive trend of frequency. The asymmetry can be used if slight tensile stress from the process integration can be obtained as it enhances the coupling coefficient.**

Keywords—piezoelectric, MEMS, frequency, FBAR, resonators, residual stress, deformation, modeling.

I. Introduction

The Film Bulk Acoustic Resonators (FBAR) consists of a piezoelectric layer sandwiched between two metal electrodes [1]. FBAR has served as a crucial building block in the design of filter applications for 5G applications at high frequencies [2]. The introduction of in-plane residual stress is an important design consideration for FBAR applications such as oscillators [3]. The residual stress is introduced in the microstructures during the microfabrication process [4]. They are defined as the stress which is present in the elastic layer without the presence of any external impulse. The residual stress results in deformation, fracture, creep, fatigue, and other changes to the structure. These consequences of the residual stress can affect the performance of the FBAR. For Aluminum Nitride (AlN) or Scandium Aluminum Nitride (ScAlN), generally, compressive stresses are introduced [5]. This compressive stress results in the stack having deformation [6]. The variation of the residual stress value in the AlN film which is widely used for FBAR depends on the thickness of the film [6]. The in-plane residual stress can impact the geometric and material properties of the piezoelectric layer. The impact of

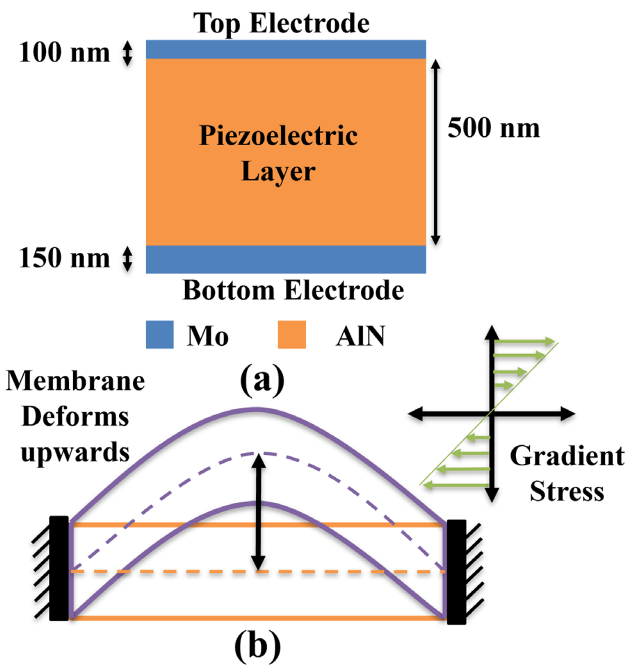

Figure.1 (a) The schematic cross-section of the FBAR stack. (b) The schematic shows the deflection of the membrane under the effect of residual stress.

the residual stress on the piezoelectric constant (e_{33}) has been shown by previous works [7]. The effect of variation of the bottom electrode shows that the use of different materials can also have an impact on FBAR performance [8]. Huang et. al [9] provided some analytic models to predict the dependence of initial stress on FBAR performance. But no previous work analyzes the effect of asymmetry of the top and bottom electrode and the deformation that affects the FBAR performance. This work will segregate the individual impacts of in-plane residual stress due to asymmetry and material property using FEM simulation.

II. Modeling the Impact of In-Plane Stress

Fig. 1(a) shows the schematic of the material stack that was considered for the simulation of the FBAR. Fig. 1(b) presents the schematic of the nature of deformation post the FBAR fabrication. The FBAR in this work uses a 500 nm AlN piezoelectric layer employing Molybdenum of thickness 100 nm and 150 nm as top and bottom electrodes, respectively. The effect of residual stress on the FBAR structure experimentally is shown in Fig. 2 by optical profiler image It shows the deformation post-fabrication in the FBAR membrane. To correlate this variation of resonant frequency in measurement, simulations were performed to take the effect of stress stiffening on FBAR with unequal/equal top and bottom electrode thickness, and piezoelectric constant (e_{33}) of the AlN film.

A. FEM simulation to correlate experimental deformation

To correlate the experimental deformation, the FEM simulation provided an approximate value of the residual stress that would provide a deformation close to the experimental value as shown in Fig. 3. The FEM simulation using COMSOL 6.0 uses a two-step study. The first step is the stationary simulation that provides deformation corresponding to the initial value of stress introduced in the piezoelectric layer. This deformation can roughly provide the value of the compressive stress that results in the stack buckling up. The subsequent simulations decouple the individual impact of the stress stiffening, deformation, and material property change on the FBAR performance. In COMSOL to implement the effect of the residual stress the initial stress and strain boundary condition is used. The PML is used to provide the fixed-fixed boundary condition on two sides of the FBAR. The fixed boundary condition at the PML ends is necessary to prevent convergence errors in the FEM simulation. To include the effect of deformation from the stationary solver, the geometric non-linearity option of the frequency domain perturbation study is enabled.

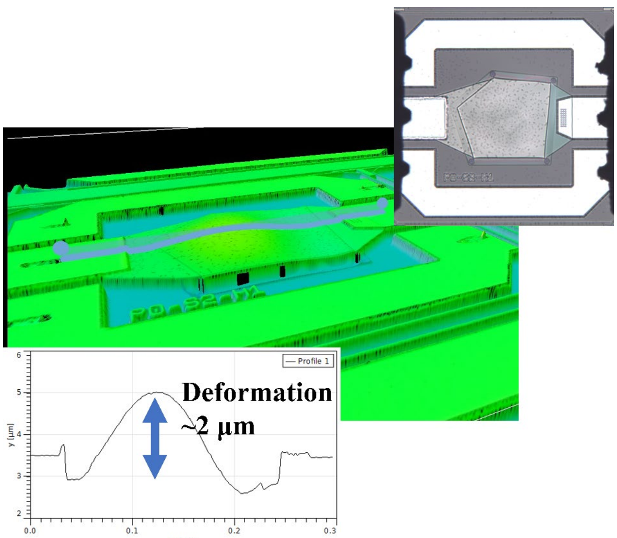

Figure. 2 The 3-D profile measurement of the FBAR with the inset showing profiling data and an optical image of the device under test (DUT).

B. Stress impact on equal electrode thickness

This case of the simulation decouples the effect of the large geometric deformation. The top and bottom electrode thickness is kept the same and equal to 100 nm. In this case, due to the symmetry, the neutral axis lies at the center of the stack thickness. Fig. 4(a) presents that the variation of the resonance frequency with the stress value shows a linear increment trend. The coupling coefficient value does not change with stress. Unlike the previous case where the trend is non-linear. Hence to have a predictive variation and keep the deformation low for FBAR, the top and bottom electrode thickness should be equal.

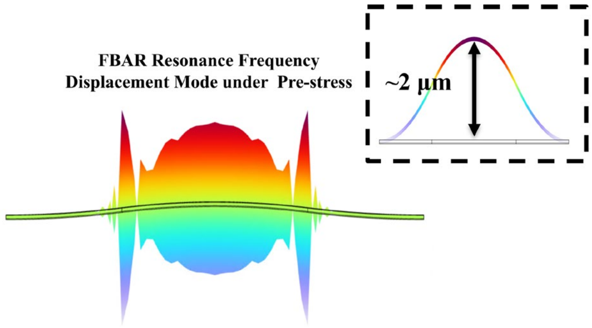

Figure. 3 The displacement mode shape under pre-stressed conditions at the resonance frequency with the inset showing the stationary simulation deformation value close to the measured value under the effect of compressive initial stress value of -550 MPa.

C. Stress impact correlated with e33 change

Tyokoyama et al [7] present the effect of in-plane stress on the piezoelectric constant of the AlN. In this part of the simulation, using the measurement data from this work, the parametric variation of the stress changes the corresponding value of e_{33}. As an FBAR is highly sensitive to the e_{33} variation, the trend in Fig. 4 (b) shows the incremental trend for both the resonant frequency and coupling coefficient. The

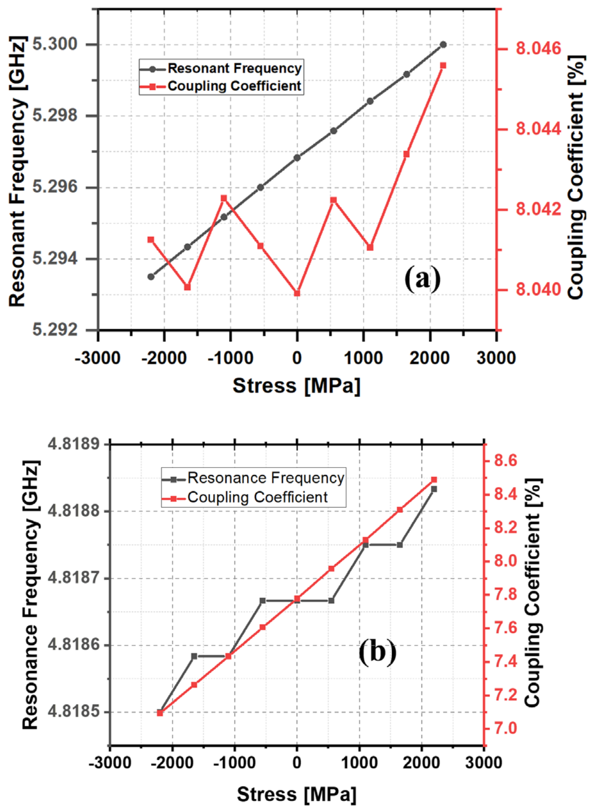

Figure. 4 (a) Impact of stress-stiffening on equal top/bottom electrode thickness, (b) Impact of correlated stress with e_{33} variation on unequal thickness.

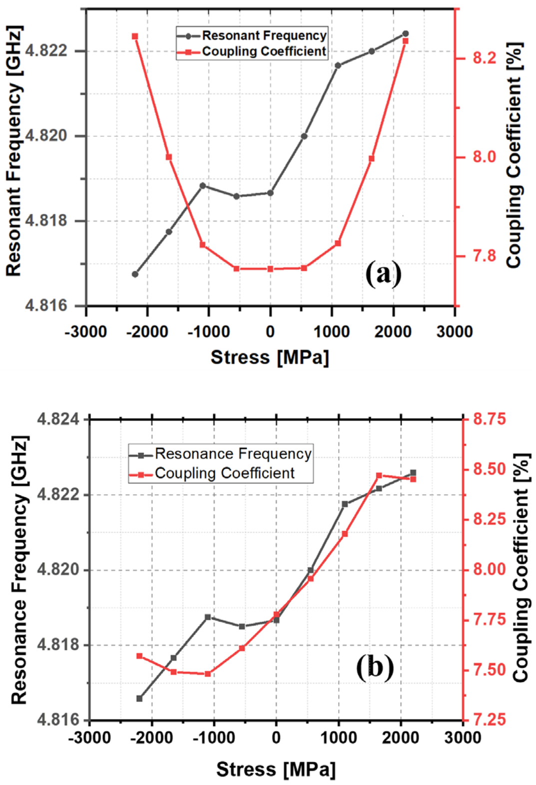

Figure. 5 (a) Impact of stress-stiffening on non-equal top/bottom electrode thickness, (b) Overall Impact of stress-stiffening and e_{33} variation on unequal top/bottom electrode thickness.

resonance frequency increases with the increase in the residual stress and the coupling coefficient also increases as the e_{33} value increases.

D. *Stress impact on unequal electrode thickness*

This simulation presents the effect of the change in the value of the in-plane residual stress on the resonance frequency of the FBAR. Fig. 5(a) shows the variation of the resonance frequency and coupling coefficient under the effect of both compressive and tensile stress. This simulation incorporates the effect of stress stiffening for the case when the top and bottom electrode thicknesses are unequal. In this case, due to the asymmetry, the neutral axis of the volumetric strain is not at the center. When residual stress is applied to such a stack it undergoes large out-of-plane structural deformation. Stress stiffening that is defined as the stiffening of the structure under the effect of applied stress. The stress stiffening should be considered in the case of thin films when the bending stiffness is very small compared to the stiffness in the axial direction. The trend shows an increase in the resonance frequency under the incremental value of stress.

Table I: Comparison of resonance frequency sensitivities variation for modeling individual impacts.

Case	**Sensitivity (Δfs/fs)/Δσ (ppm/MPa)**
Unequal electrode thickness	2.68
Equal electrode thickness	2.78
e_{33} change	0.12
Stress stiffening and e_{33} variation	2.82

E. *Stress impact including stress stiffening and e_{33} variation*

To incorporate the overall effect of the residual stress over the FBAR performance the stress stiffening and the e_{33} variation have been included in one model to combine the impact of all the variants. Fig. 5(b) shows the overall trend of the combined effect on the resonance frequency. Table I shows the sensitivities of all the cases. It can be noticed from the trend of Fig. 5(b) that the overall trend is still incremental with respect to the increment in the value of the residual stress. This trend can serve as a reference to co-simulate the device performance for any stack variation for the FBAR. The simulation methodology can be extended to other BAW devices as well.

III. Conclusion

The various trends from the individual impact modeling confirm that FBAR with symmetric stack thickness can reduce the effect of variation in coupling coefficient and provide a predictive linear trend of increasing resonant frequency with increasing residual stress. This simulation model provides a reference for what to expect from an FBAR that has large deformation. For the larger size of the FBAR membrane, the deformation will be high, as the stiffness will be lower for the larger membrane. So, to reduce the effect of residual stress the membrane size can be reduced to decrease the effect of residual stress. With more compressive stress the FBAR performance is degraded. The FBAR design should have less compressive residual stress. The stack can be optimized to have a slight tensile residual stress. Too high tensile residual stress can result in cracks even though they are enhancing performance in the design. In the future, a more comprehensive study of the residual stress impact on each layer of the stack and matching the results close to the measurement results can be done.

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References

[1] R. Ruby, "A snapshot in time: The future in filters for cell phones," *IEEE Microwave Magazine*, vol. 16, no. 7, pp. 46–59, Aug. 2015, doi: 10.1109/MMM.2015.2429513.

[2] C. Liu, M. Li, N. Wang, and Y. Zhu, "Sub-100nm Al0.7Sc0.3N Thin Films for Next Generation Bulk Acoustic Wave Resonators and Filters," Proceedings, 2022 IEEE International Ultrasonics Symposium (IUS), Venice, Italy, 2022, pp. 1-3, doi: 10.1109/IUS54386.2022.9957221.

[3] R. Ruby, S. Sridaran, S. Ortiz and K. G. Oppermann, "A comparison of FBAR oscillators with standard resonators and stress relieved resonators," *2013 Joint European Frequency and Time Forum & International Frequency Control Symposium* (EFTF/IFC), Prague, Czech Republic, 2013, pp. 754-757, doi: 10.1109/EFTF-IFC.2013.6702304.

[4] Tatsuo Tabaru and Morito Akiyama, "Residual stress reduction in piezoelectric Sc0.4Al0.6N films by variable-pressure sputtering from 0.4 to 1.0 Pa," *Thin Solid Films*, vol. 692, no. 1, pp. 137625, Dec. 2019, doi: 10.1016/j.tsf.2019.137625.

[5] Glenn Ross, Hongqun Dong, Cyril Baby Karuthedath, Abhilash Thanniyil Sebastian, Tuomas Pensala, Mervi Paulasto-Kröckel, "The impact of residual stress on resonating piezoelectric devices," *Materials & Design,* vol. 196, no. 1, pp. 109126, Nov. 2020, doi: 10.1016/j.matdes.2020.109126.

[6] Y. Song, C. Perez, G. Esteves, J.S. Lundh, C.B. Saltonstall, T.E. Beechem, JI Yang, K. Ferri, JE Brown, Z. Tang, J.P. Maria, D.W. Snyder, R.H. Olsson, B.A. Griffin, S.E. Trolier-Mckinstry, B.M. Foley, and S. Choi, "Thermal Conductivity of Aluminum Scandium Nitride for 5G Mobile Applications and beyond," *ACS Applied Materials and Interfaces*, vol. 13, no. 16, pp. 19031-19041, Apr. 2021, doi: 10.1021/acsami.1c02912.

[7] T. Yokoyama, Y. Iwazaki, T. Nishihara and M. Ueda, "Analysis on electromechanical coupling coefficients in AlN-based bulk acoustic wave resonators based on first-principle calculations," 2012 IEEE International Ultrasonics Symposium, Dresden, Germany, 2012, pp. 551-554, doi: 10.1109/ULTSYM.2012.0137.

[8] Jin-Bock Lee, Jun-Phil Jung, Myung-Ho Lee, Jin-Seok Park, "Effects of bottom electrodes on the orientation of AlN films and the frequency responses of resonators in AlN-based FBARs," *Proceedings of the 30th International Conference on Metallurgical Coatings and Thin Films 2004*, pp. 610-614, doi: 10.1016/j.tsf.2003.07.023.

[9] D. -j. Huang, X. -y. Luo and J. Wang, "Influence of initial stresses on resonance properties of FBAR," *2012 Symposium on Piezoelectricity, Acoustic Waves, and Device Applications* (SPAWDA), Shanghai, China, 2012, pp. 144-147, doi: 10.1109/SPAWDA.2012.6464056.