Iterative Analysis Approach using interactive Python-FEM to estimate the residual stresses in PMUTs

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Abstract—**Key performance metrics of Piezoelectric Micromachined Ultrasonic Transducers (PMUTs), such as resonance frequency (f_r) and electromechanical coupling k_t^2, are significantly impacted by the residual stress. In this study, we present an iterative analysis approach that utilizes interactive Python-FEM to estimate residual stress in PMUTs by integrating optical profile data with a finite element model (FEM) employing Newton-Raphson approximation. The proposed approach is validated using a known solution obtained from COMSOL simulation. We successfully applied this approach to estimate residual stress in three PZT PMUT samples fabricated in a Lab-in-Fab (LiF) facility. The estimated residual stresses are -171 MPa, -111 MPa, and -169 MPa indicate a compressive nature and align with the optical profile data. These values fall within the process condition range for the LiF physical vapor deposited (PVD) lead-zirconate-titanate (PZT) PMUT process.**

Keywords— PMUT; residual stress; PZT; interactive iterative approach; MEMS; FEM; Python

I. INTRODUCTION

PMUTs have attracted considerable attention in a wide range of ultrasonic applications, including fingerprint sensing, non-destructive testing, proximity sensing, gesture control and medical imaging. The advancements in microelectromechanical systems (MEMS) fabrication technology have led to the development of high-performance piezoelectric materials like scandium (Sc) doped aluminium nitride (AlN) and sputtered PZT. PMUTs are typically consist of multilayers for piezoelectric actuation and sensing. Recently, it has been reported that the residual stress in these layers has significantly affect the key performance metrics, such as the resonance frequency (f_r) and electromechanical coupling (k_t^2). Ross *et al.* reported a range of residual stress variation along the wafer in AlN PMUTs, with values spanned a range of -357 MPa to -56 MPa. This led to a corresponding variation in fr, ranging from under 400 kHz to over 600 kHz [1]. Jihang et al. demonstrated significant changes in k_t^2 at the wafer level, with deviations spanning from 0.5% to 3% with respect to the local residual stress in PZT PMUTs [2]. The observed variation in the f_r of the devices fell within the range of 157 kHz to 215 kHz.

Equivalent circuit models [5,6] and analytical models [7,8] have been developed to evaluate the residual stresses. But these models become challenging to employ for complex geometries with multilayered structures. Experimental method using X-Ray Diffraction (XRD) was demonstrated to extract in-plane biaxial residual stress in PMUTs capturing both local and global stresses across a wafer [1]. This approach accurately estimates the residual stress, but it requires complex data analysis with specialized instruments. FEM [9,10,11,12] is one of the most popular approach due to its ease of use and capability for analysing coupled Multiphysics problems, complex geometries, and multilayer structures. However, it requires extensive manual parametric study to correlate FEM solution with measurement data. In this work, we propose a Python-FEM interactive analysis approach to estimate residual stress in PMUTs by efficiently combining the optical profile data with FE model using Newton-Raphson approximation. The proposed approach is validated by using the known solution which was obtained from COMSOL simulation and then successfully applied to evaluate the residual stress in three PZT PMUT samples.

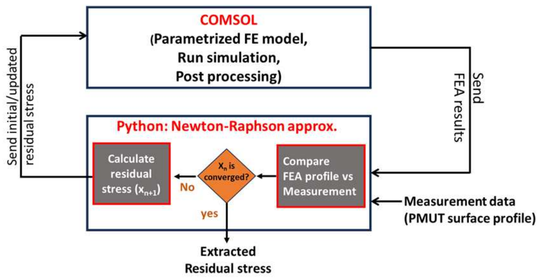

Fig. 1. Schematic of the interactive iterative approach.

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Initial condition (PZT stress in MPa) @ n=0→	**200**		**100**		**-300**		**-400**	
Iteration ↓	Stress (MPa)	Error	Stress (MPa)	Error	Stress (MPa)	Error	Stress (MPa)	Error
1	-325.2106	1.58e-3	-156.4121	1.21e-3	-500.0000	1.84e-3	-9.3278	1.396e-3
2	-48.9364	1.11e-3	-97.0671	3.21e-4	-115.3153	9.47e-4	-100.1890	1.142e-5
3	-98.6504	3.29e-4	-99.8871	2.40e-5	-99.7955	8.61e-5	-100.0007	6.102e-6
4	-99.9893	1.43e-5	-99.9954	6.41e-6	-99.8545	7.35e-6	--	--
5	-100.0007	6.10e-6	--	--	-100.0008	6.10e-6	--	--
Ref. Solution (MPa)	-100		-100		-100		-100	
Relative Error (%)	7.791e-04		4.583e-03		7.797e-04		7.789e-04	

Table 1. Convergence properties of the proposed approach at different initial conditions compared with respect to the COMSOL reference solution.

II. ITERACTION BASED INTERACTIVE METHOD

The proposed approach consists of two parts: a parametrized FEM using COMSOL 6.1, and an iterative Newton-Raphson approximation algorithm [13,14]. implemented in Python, shown in Fig. 1. The algorithm performs FE simulation iteratively by comparing the simulated displacement caused by initial/updated residual stress with the measured optical profile data, which represents the displacements due to residual stress in PMUTs. Initial and updated (after each iteration) stress values with polarity (whether compressive or tensile) from Python were sent to COMSOL structural mechanics model to iteratively process the measured data until the FE simulated displacement converges with the displacement from the measured optical profile data of a PMUT. The Newton-Raphson approximation equation implement in Python is given in Eq. (1),

$$\boldsymbol{x_{n+1}} = \boldsymbol{x_n} - \frac{\boldsymbol{f(x_n)}}{\boldsymbol{f'(x_n)}} \tag{1}$$

where $\boldsymbol{x_{n+1}}$ is the new updated stress value, $\boldsymbol{x_n}$ is the previous iteration stress value, the function $\boldsymbol{f(x_n)}$ corresponds to the calculation of the error between the previous iteration solution and the refences solution, the derivative of $\boldsymbol{f(x_n)}$ which is $\boldsymbol{f'(x_n)}$ used to approximate the slope of the error function. This can be extended to multi variable parameter evaluation.

III. PMUT MODEL FOR FEM

A one-port circular PVD PZT PMUT with membrane diameter of ~600µm and PZT of diameter 420µm is fabricated using MEMS process [2] in our LiF 8-inch line. As shown in Fig. 2, a 2µm thick sputtered PZT is sandwiched between two platinum electrodes on a 4µm Si and 0.5µm SiO_2 elastic membrane. A parameterized 3D FEM model is developed in COMSOL to receive initial/updated stress values from Python through method call functions.

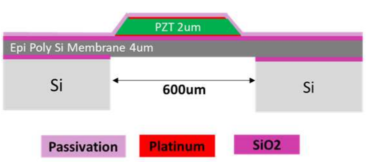

Fig. 2. Cross-sectional view of a PVD PZT pMUT.

IV. RESULTS AND DISCUSSION

A. *Basic Validation of the proposed method against COMSOL reference solution*

The accuracy of convergence of our proposed approach is demonstrated by validating the interactive method with different initial stress values (for first iteration) applied to the piezoelectric layer of our symmetric three-dimensional model (Fig. 3a) in COMSOL solution and obtaining same at a given stress in piezoelectric layer with initial conditions, shown in Fig. 3 and Table 1. For any given initial condition, the iterative solution converge to the refence solution, typically within 4 to 5 iterations as shown in Table. 1.

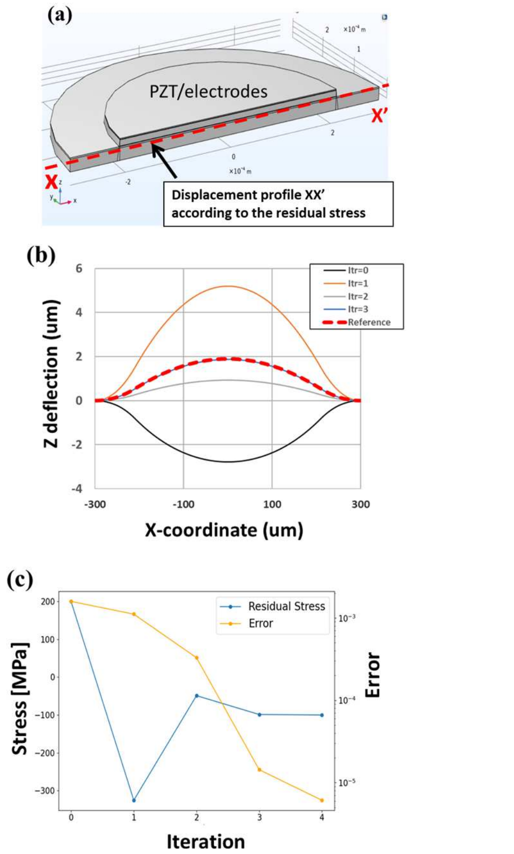

Fig. 3. (a) Symetric 3D COMSOL model: line X-X' is the data collection line (b) Membrane displaements vs iterations compared with reference COMSOL solution (c) Stress and error convegence respect to reference solution (PZT stress = -100MPa) from COMSOL for initial condition of 200MPa in PZT layer

B. *Evalation of residual stress in fabricated PZT PMUTs*

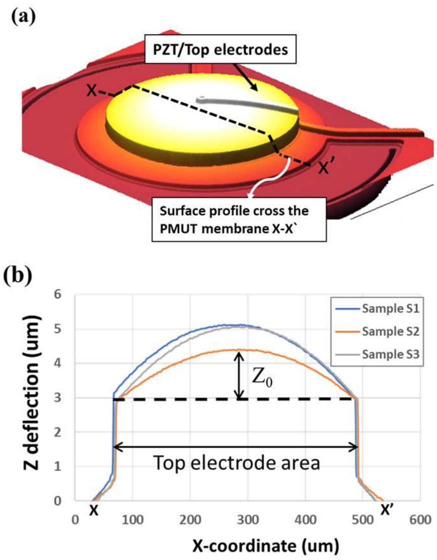

Fig. 4, (a) Top view of optical profile image of PMUT: line X-X' is the data collection line (b) topography of a membrane of three PVD PZT PMUT samples: S1, S2, & S3

The proposed approach is employed to evaluate the residual stress in actual fabricated PZT PMUTs. The surface optical profile scan along the line X-X' shown in Fig. 4(a) is depicted in Fig. 4(b), which was collected for three samples: S1, S2, and S3. In the initial unbiased state, the membrane shows an upward deformation. This indicates that the overall residual stress is compressive in nature. The deflections, Z_0, of the piezo stack measured at the centre of the membrane were 2.26µm, 1.41µm and 2.16µm for PMUTs on samples S1, S2, and S3, respectively. The optical profile data shown in Fig. 4(b), will serve as a refences solution in the Python script. The Newton-Raphson approximation algorithm compares the optical profile displacement data with the COMSOL simulation displacement solutions. It iteratively updates the PZT stress value in the COMSOL simulation based on the error between the FEA solutions and the measurement solution. This iteration process continues until the FEA and measurement solutions are converged. The error function defined in Python computes the error between the fitted optical profile Z-displacement of full PMUT membrane cross section (X-X') shown in Fig. 4(a-b) versus the deformation profile obtained from the COMSOL simulation. Fig. 5 shows that the FEA and measurement solutions are converged within 5 iterations. The estimated residual stresses for samples S1, S2, and S3 are approximately -171 MPa, -111 MPa, and -169 MPa, respectively, as shown in Fig. 5(a). These values are in the range of process condition for LiF PVD PZT PMUT process, indicate that the residual stresses are compressive in nature. This result aligns with the optical profile data, where the upward bending of the membrane indicates compressive stress. Further, the maximum residual stress is observed in samples S1 and S3 compared to S2, which correlates with the membrane centre deflections (Z_0). The deflections of S1 and S3 are greater than that of S2, suggesting a relationship between the initial bending and residual stress.

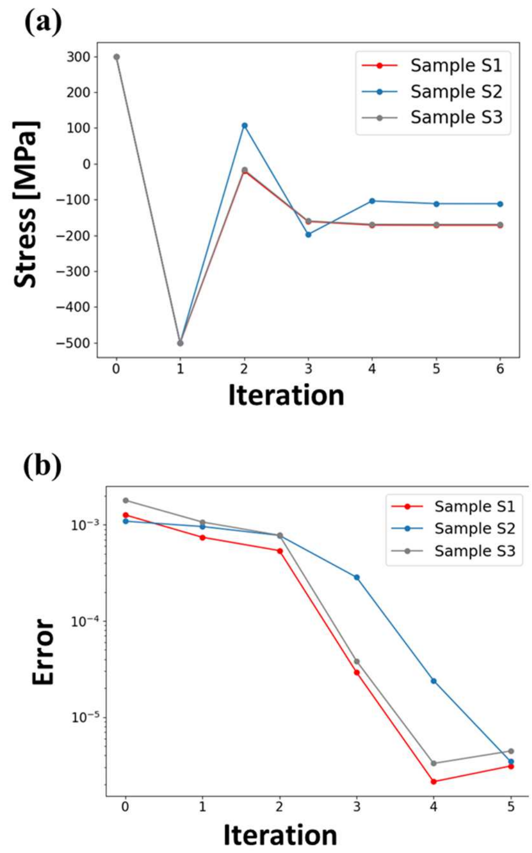

Fig. 5. Convergence properties of the proposed approach with respect to optical profile results of three PVD PZT PMUT samples: S1, S2, & S3, (a) Convergence of residual stress V/s iterations, (b) error V/s iterations.

V. Conclusions

We have presented an iterative analysis approach using interactive Python-FEM to estimate the residual stress in PMUTs. By coupling the FEM and a Newton-Raphson approximation algorithm in Python, our approach iteratively compares simulated displacements with measured optical profile data to estimate the residual stress in PMUTs. We have successfully applied our proposed approach to estimate the residual stress in three PZT PMUT samples (S1, S2, and S3) fabricated in LiF. The estimated residual stresses (-171 MPa, -111 MPa, and -169 MPa) indicate a compressive nature and align with the optical profile data. Further, we have validated the accuracy of our approach by demonstrating convergence with a reference COMSOL solution for different initial stress conditions. This approach will be extended to estimate multilayer residual stress. This interaction can be extended to extract d_{31} coupling coefficients of piezoelectric films of various complex geometrical direction.

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