FINITE ELEMENT ANALYSIS OF FABRICATION RELATED THERMAL EFFECTS IN CAPACITIVE MICROMACHINED ULTRASONIC TRANSDUCERS

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Abstract – **The accurate prediction of the static operation point of capacitive micromachined ultrasonic transducer (CMUT) membranes is essential for dynamic performance modeling, device design, and device fabrication. We evaluate whether fabrication-related stress effects in CMUT cells cause significant deviations observed between membrane deflection measurements and calculations. Our finite element analysis (FEA) considers the thermal structural interaction associated with the temperature stress history during device fabrication. Specific boundary conditions enable thermal expansion in all directions. Compared to conventional FEAs with one static solution step, we use seven static solution steps using the element birth and death feature of ANSYS to assemble the CMUT cell layer by layer at the appropriate deposition temperatures. We use measured static deflection profiles of metallized and non-metallized membranes with different diameters and thicknesses to extract all unknown parameters for the model. This approach improves the prediction of membrane deflections significantly, and it explains why present models often overestimate the collapse voltage.**

I. INTRODUCTION

In a vacuum sealed CMUT cell, the ambient pressure and the DC bias voltage, which is applied during device operation, contribute to the static membrane deflection. When the sacrificial release method [1] is used to fabricate the device, the inherent residual stress [2]–[4] of the deposited film (low-stress silicon nitride layer) also influences the membrane deflection.

The accurate prediction of the static membrane deflection is essential for all subsequent dynamic performance modeling steps in FEA. That is to say that only if the model is capable to determine the static operation point of the CMUT membrane correctly, the modal, harmonic, or transient simulation runs, all prestressed, will give results, worth to be compared directly to measurement results. This especially applies to the accurate prediction of the collapse voltage, which is an important criterion for the design and operation of a CMUT.

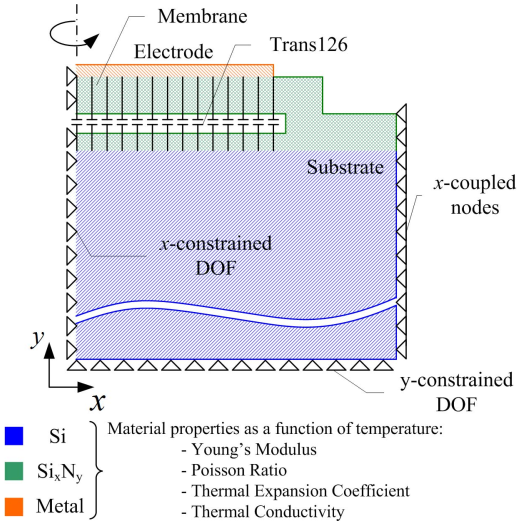

Fig. 1. Schematic of the thermal-structural finite element model (FEM) for the calculation of the static operation point of circular CMUT cells.

In our recent work we observed a significant discrepancy between the calculated and measured collapse voltages. This brought into question whether our finite element models include all driving physical effects, besides ambient pressure, bias voltage, and residual stress. For example, we calculated the collapse voltage to be 58 V, however, the measurements revealed a value of 20 V. Although charging effects might be an explanation for this discrepancy or at least a significant part of it, this paper shows that charging effects are not the only reason why present FEA often overestimate the collapse voltage. The lack of fabrication related thermal stress effects in present FEAs is one of the main reasons why the static operation point of CMUT membranes is often calculated inaccurately. In this paper, we exclude all uncertainties regarding charging effects by focussing on the direct comparison between calculated and measured static membrane deflections. The CMUT cells used for this purpose never had an electrical DC bias voltage applied before these deflection measurements were taken.

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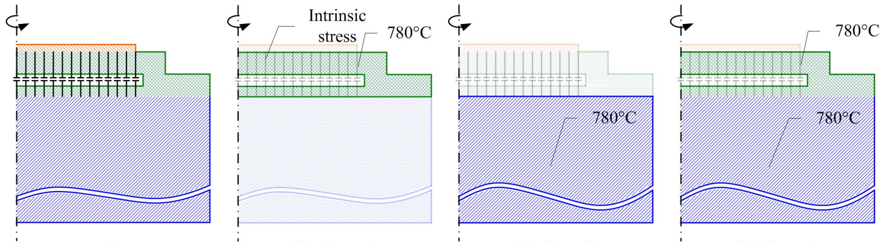
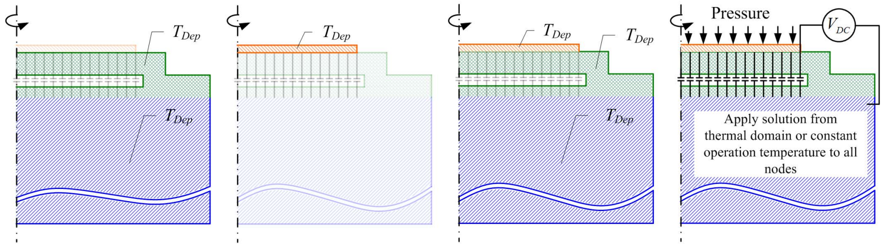


(a) (b) Step 1 (c) Step 2 (d) Step 3



(e) Step 4 (f) Step 5 (g) Step 6 (h) Step 7

Fig. 2. Illustration of how the element birth and death feature of ANSYS is used to assemble the CMUT cell layer by layer in seven steps in the solution part of the FEA. The parts of the structure, which are illustrated in a transparent fashion in this figure, only consist of elements, which are all killed during the specific solution step.

II. THERMAL-STRUCTURAL FEA FOR CMUTS

In addition to the commonly used electrical-structural domain, our FEA is characterized by an extension into a thermal domain with its main consequence of thermal expansion. Therefore, the FEA is able to consider fabrication related thermal stress effects in CMUTs.

Our FEM (Fig. 1) represents the most used structure for CMUT cells, when fabricated with the sacrificial release method [1]. Because the test devices fabricated for verification purpose only had circular cells, an axisymmetric 2D model can be used as good approximation. However, the same thermal-structural domain extension can be applied easily to more sophisticated 3D models for all other cell shapes. Compared to other FEAs, our model is distinguished by the following four features: First, the whole substrate (500 μm of silicon) below the membrane is modeled; Second, all related material properties (Fig. 1) are put into the model as a function of temperature. These properties need to be specified over a large temperature range, *i.e.* up to the maximum temperature that occurs during the device fabrication; Third, the model has very specific boundary conditions, that enable the whole structure to expand or contract in both x and y direction when a thermal load is applied (Fig. 1). The nodes on the bottom side of the substrate are only constrained in x-direction to allow the model to expand or contract in y-direction. The nodes at the right side of the model are all coupled to move only the same amount in x-direction by using a master degree of freedom [6]. Coupling these nodes mimics an infinite extension of material around the circular cell, which is required because of the transition from the silicon to the silicon nitride layer; Fourth, instead of only one solution step in the solution part of the FEA, seven steps that mimic the fabrication process (7-step model), are used. This last feature is described in more detail in the rest of this section:

In the seven solution steps of the 7-step model, the element birth and death feature (ekill, ealive [6]) of ANSYS is utilized to assemble the CMUT cell layer by layer at the related deposition temperatures (Fig. 2). Killing an element before a solution step means that the stiffness matrix of that element is multiplied by a small multiplication factor (10^{-6} by default), which deactivates the element for this solution step. The order of the steps reflects the situation according to the two main events during the device fabrication concerning thermal stress effects. These two main events are a silicon nitride deposition and a metal (aluminum) deposition step. The silicon nitride layer is built by all together three depositions at 780 °C in a low-stress LPCVD step with two intervening fabrication steps to define the gap, *i.e.* a poly silicon deposition (sacrificial layer) and a potassium hydroxide (KOH) step (releasing the membrane). These five fabrication steps are approximated in the model by assuming that the silicon nitride membrane is completely formed in one single fabrication step, which is modeled by solution steps 1, 2 and 3 (Fig. 2). The metal deposition step to build the electrode is done at a specific deposition temperature T_{Dep}, which requires the solution steps 4, 5, and 6 (Fig. 2). The ambient pressure, the DC bias voltage, and the operating temperature of the CMUT are applied in the seventh and final solution step, which reveals the static operation point of the CMUT cell, *i.e.* the static membrane deflection.

III. MODEL PARAMETER EXTRACTION

Before the FEA can be verified by a comparison of calculated and measured membrane deflections, all related material properties and fabrication related deposition temperatures need to be determined. The Young's modulus and the Poisson ratio of the low stress silicon nitride, which we deposited in a LPCVD tube at the Stanford Nanofabrication Facility (SNF), are known from previous work [5]. In this context, the unknown parameters are the coefficient of thermal expansion (CTEX) and the intrinsic stress of the low stress silicon nitride, as well as the temperature of the membrane during the metal deposition step, *i.e.* T_{Dep} (Fig 2).

The basic idea of how to extract these three parameters is to measure both the static membrane deflections before and after the metal deposition step. Thus, the problem to determine all three unknown parameters can be split up in two simpler tasks (Fig. 3, optimization 1 and optimization 2): First, the parameters for the intrinsic stress and the coefficient of thermal expansion of the silicon nitride were adapted in an optimization run for best average fit to the membrane deflection measurement results obtained before the metal deposition step; Second, the temperature of the membrane during the metal deposition (T_{Dep}) was adapted for best average fit to the measurements, obtained after the metal deposition step. For both optimization runs, we used 12 representative cell geometries on the wafers fabricated, *i.e.* cell diameters of 24, 30, and 36 μm and membrane thicknesses from 400 to 900 nm. The deposition thickness of the aluminum (half-metallization) ranged from 100 to 300 nm. A white light 3D surface profiler (New View 100, Zygo Corporation, Middlefield, CT) was used to measure the static membrane deflection profiles under the atmospheric pressure of 1 atm.

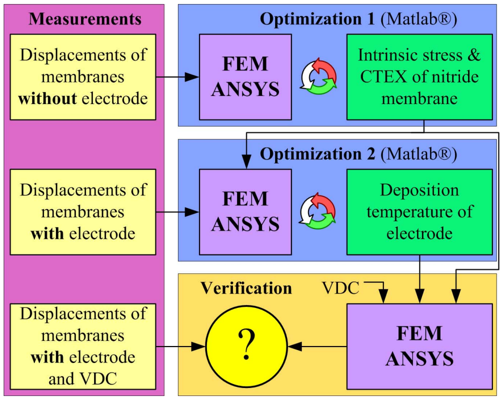


Fig. 3. Illustration of how all unknown model parameters are extracted in two subsequent optimization runs, using two sets of membrane deflection measurement data, obtained before and after the metallization step.

IV. RESULTS AND VERIFICATION

The result of the first optimization run (Fig. 3) shows that the low stress silicon nitride has a 7.9% larger CTEX value than of silicon and that the intrinsic stress in the membrane is 84 MPa tensile. As expected, using these two parameters in the FEA improves the prediction of the membrane center deflection before the metal deposition step significantly from -31.8% ($\sigma = 16\%$) to 0.4% ($\sigma = 10.3\%$), as depicted in Fig. 4.

The second optimization run (Fig. 3) determines an average metal deposition temperature (T_{Dep}) of 62.3 °C ($\sigma = 21.4$ °C), which gives the best average fit (orange curve, Fig. 5) to the measurement results for various cell geometries, i.e. three different groups of cell diameters (24, 30, and 36 μm).

However, for small center deflections, *i.e.* cells with a diameter of 24 μm, the model overestimates the static center deflections. For large center deflections (36 μm cells) the model underestimates the deflections. The reason for these deviations seems to be that CMUT cells with larger diameters heat up more during the metal deposition step, especially in the center region of the membrane. Note that the cells are vacuum sealed and the main heat flow between membrane and substrate happens at the post region of the cell. If the optimization run (Fig. 3) is done for three separate groups, *i.e.* for 24, 30, and 36 μm diameters, this assumption is supported and the FEA can be further improved. The optimum value for T_{Dep} is 82.6 °C ($\sigma = 21.6$ °C), 61.0 °C ($\sigma = 9.18$ °C), and 43.1 °C ($\sigma = 9.31$ °C) for 36 μm, 30 μm, and 24 μm cell diameters, respectively.

It is clear from Fig. 5 that after the metalliza-

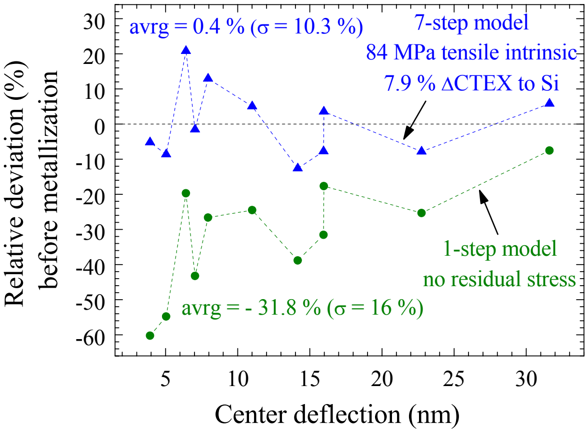


Fig. 4. Relative deviations between measured and calculated static membrane center deflections, for different cell geometries, before the metal deposition step. Each data point corresponds to a certain cell geometry.

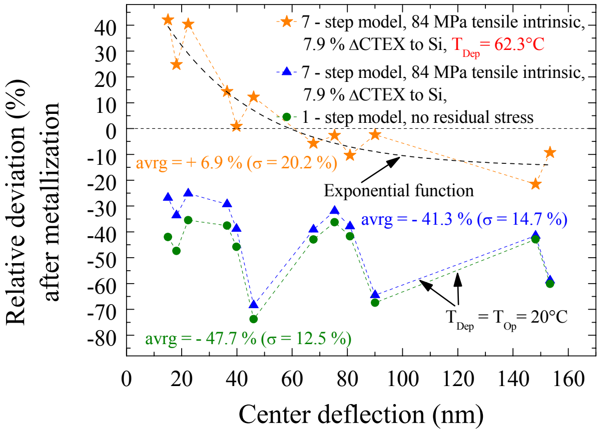


Fig. 5. Relative deviations between measured and calculated static membrane center deflections, for different cell geometries, after the metal deposition step (aluminum, half-metallization). Three models with different parameter sets are compared

tion step, the thermal stress between the aluminum electrode and the silicon nitride membrane is the main reason why present FEAs underestimate the static membrane deflections (green curve, Fig. 5), and, therefore, overestimate the collapse voltage. This is even valid when these models consider the residual stress in the silicon nitride membrane (blue curve, Fig. 5). Further, it is worth to mention that these cells never had an electrical DC bias voltage applied before these profile measurements, which shows that charging effects are not required as explanation to why present models often underestimate the membrane deflection and therefore overestimate the collapse voltage.

V. CONCLUSION

This paper demonstrates that present FEAs do not consider all physical effects that have significant influence on the static membrane deflection. The lack of fabrication related thermal stress effects in present FEAs is one of the main reasons why the static operation point (static membrane deflection) of CMUT cells is often calculated inaccurately. Further, our results explain why present FEAs overestimate the collapse voltage. The main part of the improvement concerning the prediction of the static center deflection (88%) comes from the fact that the model considers the thermal expansion coefficient mismatch between the aluminum electrode and the nitride membrane. For "thermal-stress-sensitive" CMUT designs (large cell diameters, thin membranes, small gaps, thick electrodes, not full metallized), metals other than aluminum as CMUT electrode material should be considered, *e.g.* a titanium base layer with a platinum electrode. Further, our model predicts that full metallized cells are less sensitive to stress effects related to the thermal mismatch between the electrode and membrane and it is suitable for investigations of the CMUT behavior at different operation temperatures.

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