

Air-Coupled PMUT at 100 kHz with PZT Active Layer and Residual Stresses: Multiphysics Model and Experimental Validation

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Abstract

In this paper a complete Multiphysics modelling via the Finite Element Method (FEM) of an air-coupled Piezoelectric Micromachined Ultrasonic Transducer (PMUT) is described, with its experimental validation related to the mechanical and acoustic responses.

The numerical model takes into account the presence of fabrication induced residual stresses, which determine a non-linear initial deformed configuration of the diaphragm and a substantial frequency shift associated with the fundamental eigenmode of the vibrating system.

The complete simulation of the device's behaviour is obtained considering multiple coupling between different fields: electro-mechanical coupling for the piezoelectric model, thermo-acoustic-structural interaction and thermo-acoustic-pressure interaction for the waves propagation in the surrounding fluid.

The model gives a realistic estimation of the fundamental frequency and of the PMUT's quality factor through the adoption of large deformation analyses and by means of a proper modelling of the air, considering its thermo-viscous properties, that induce the power dissipation in the so-called boundary layer at the fluid-structure interface.

The results of the numerical multi-physics model are compared with experimental ones in terms of the initial static pre-deflection, of the membrane center vertical displacement frequency spectrum and of the sound intensity at 3.5 cm on the vertical direction of the axisymmetric axis of the diaphragm.

1. Introduction

The use of piezoelectric materials in *smart* microsystems is continuously increasing, with different possible uses of both *direct* and *indirect* effects. The latter is applied for actuating purposes, e.g. in the case of micropumps [1]; *direct* effect is used e.g. for energy harvesting [2]. In the case of MEMS, some recent developments allowed for the introduction of layered structures with thin films of piezoelectric material, namely lead zirconate titanate (PZT) or aluminium nitride (AlN) [3].

Piezoelectric micromachined ultrasonic transducers (PMUTs) are layered membranes with a piezoelectric

active layer used for emitting and receiving ultrasonic waves [4]. They are widely employed for many practical purposes: medical acoustic imaging and hydrophones exploit the in-water wave propagation of ultrasonic pulses; finger-printing recognition [5] and range-finders use the in-air propagation [6]. Further applications are represented by non-destructive testing, velocity sensing and 3D obstacle recognition.

This paper builds up on a previous work [7] and deals with a new PMUT diaphragm with operational frequency of 100 kHz; experimental results are shown in the mechanical and in the acoustic domains. The attention is focused on the study of the behaviour of a single circular fully-clamped air-coupled PMUT (Fig. 1) with radius of 440 μm , aspect ratio (radius/thickness) of 55, over a fluid filled closed cylindrical cavity with height of 400 μm and same radius of the upper diaphragm. The piezoelectric active layer is made up of PZT, it is deposited with Sol-Gel technique in circular configuration with radius of 308 μm , with the center coincident with the one of the membrane.

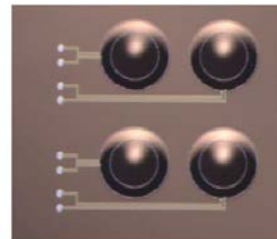


Figure 1: Optical microscope image of four PMUTs.

2. Numerical modelling

In this section a numerical finite elements model built in COMSOL Multiphysics 5.2 is presented. An axisymmetric configuration is considered, to simulate the complete behaviour in the static and dynamic regime of the device surrounded by the fluid, reducing the computational burden.

The numerical model incorporates four physics and their mutual interactions, namely: solid mechanics model of the membrane, piezoelectric effect in the PZT active layer, thermo-viscous acoustics model for the fluid near to

the vibrating diaphragm and pressure acoustics model for the fluid far from the membrane.

Each layer of the PMUT is considered as linear elastic and it is characterized by a certain amount of pre-stress acting in the radial direction of the geometry meridian plane, induced by the fabrication processes.

In the piezoelectric active layer the electro-mechanical coupling is enforced through a linear Stress-Charge constitutive relation.

Furthermore, to take into account the structural damping effect (which incorporates the anchor losses, the surface layers and the thermo-elastic losses) an isotropic structural loss factor is introduced as the inverse of the structural quality factor Q_{struct} .

The laminate system plus the cavity are inserted into a spherical thermo-viscous domain of radius equal to the wavelength $\lambda = v_s/f_0$. v_s is the sound velocity in the air at the reference state of $T_{ref} = 293.15$ K and $P_{ref} = 1$ atm, f_0 is the operational frequency of the system, that coincides with the membrane fundamental natural eigenfrequency to maximize the acoustic efficiency.

In the spherical thermo-viscous domain, the full set of equations for a compressible viscid thermally conductive fluid are solved, namely: the momentum balance equation, the mass balance equation and the energy balance equation. It is necessary to adopt such modelling for the membrane surrounding fluid due to the fact that the maximum amplitude of vibration is comparable to the thickness of the diaphragm [8-9]. The model gives an estimation of the fluid losses acting in the boundary layer above and below the vibrating membrane together with complete fluid-structure interaction for the wet boundaries.

The acoustic phenomenon far from the emitting source can be considered as an isentropic process, characterized by zero energy dissipation. To reduce the degrees of freedom of the complete system, a spherical pressure acoustic domain of thickness 4λ is modelled outside the thermo-viscous one. In this region the lossy Helmholtz equation for the pressure acoustic field is solved, considering the attenuation properties of the fluid through the Stokes' attenuation factor for the viscous and thermally conductive case [10].

Finally, outside the pressure acoustic domain, to simulate the wave radiation into an infinite medium, a Perfectly Matched Layer (PML) of thickness equal to λ is inserted.

The numerical electro-thermo-structural-acoustic response is computed after a sequence of simulations. An initial non-linear solid mechanics static analysis is performed to provide the pre-deflected configuration induced by the fabrication residual stresses, this is necessary due to the high aspect ratio of the diaphragm. An electro-mechanical static analysis in the presence of the previously computed non-linear deformation is performed to take into account the static voltage applied in the actuation phase. Finally, an electro-mechanical-acoustic analysis is performed in the frequency domain to

simulate the behaviour of the entire system, under the harmonic voltage perturbation and taking into account the non-linearities introduced before.

3. Results and experimental validation

The results of the first study described in the previous section are presented in Fig. 2: the initial static deflection of the layered system, due to residual stresses, is characterized by a typical membrane-like shape. The maximum vertical displacement is in the center of the membrane and the measured value is $5.5 \mu\text{m}$, while the corresponding numerical value is $5 \mu\text{m}$. The mismatch is attributed to the uncertainty in the values of the residual stresses.

Together with the initial deformed shape, the residual stresses have another important effect: as a matter of fact, their contribution to the geometric stiffness of the membrane changes significantly the fundamental natural frequency of the PMUT. The same vibrating system in terms of geometry and materials, without the pre-stress state, presents a theoretical value of the fundamental natural frequency of 111.5 kHz, considering the contribution to the stiffness induced by the static voltage applied through the electro-mechanical coupling. Taking into account the pre-stresses it shifts to 99.8 kHz and this is correctly captured by the numerical model which reports a value of 100.2 kHz. In order to demonstrate the shift, a frequency spectrum analysis is conducted with applied static voltage of 3 V and a harmonic perturbation with voltage amplitude of 3 V. The complete numerical electro-mechanical-acoustic frequency sweep simulation runs in 40 minutes with i7 CPU @3.4 GHz and 16 GB RAM. The experimental proof is performed by means of an oscilloscope, providing the desired voltage excitation, and by the Polytec MSA-500 Micro System Analyzer to measure the vibration of the membrane. The comparison between the two normalized vertical displacement spectra is reported in Fig. 3.

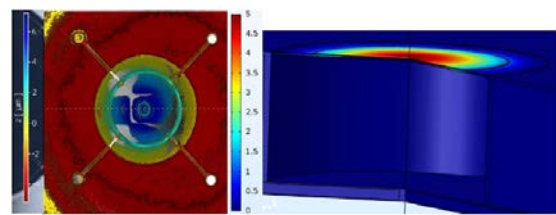


Figure 2: Initial static deflection due to fabrication residual stresses: experimental measurement by means of Polytec MSA-500 (left), numerically computed by means of COMSOL Multiphysics 5.2 (right).

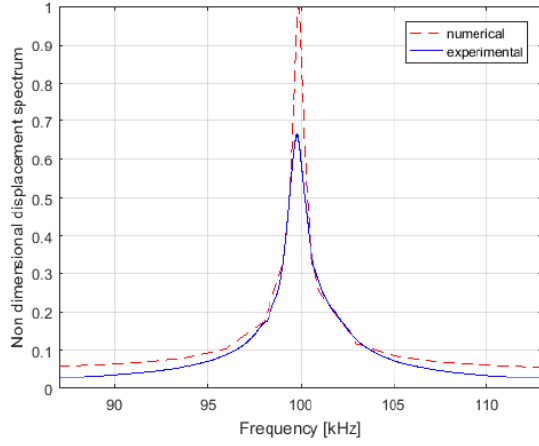


Figure 3: Normalized vertical displacement spectra for the center point of the membrane: experimental measurement by Polytec MSA-500 (blue solid line) and numerical estimation by COMSOL Multiphysics 5.2 (red dashed line).

The Q-factor is measured by means of a free vibration decay test and its value is $Q_{tot} = 80$. This device Q-factor depends on several sources of energy losses: structural losses Q_{struct} , such as thermoelastic, support, surface layer losses, and fluid losses Q_{fluid} , related to the energy radiation into an infinite medium and to the thermo-viscous losses in the air. By means of the thermo-acoustics modelling adopted for the fluid domain, it is possible to define, at least numerically, the amount of this last factor as $Q_{fluid} = f / f_{bw}$ where f_{bw} is the 3 dB bandwidth at the resonance frequency f , which results equal to $Q_{fluid} = 190$. The fluid region in which the thermal and viscous losses are greater is the so-called boundary layer, which surrounds the diaphragm on the two sides above and below. The thickness of this layer is related to the penetration depths and it is shown in Fig. 4, where the map of the total power dissipation density is reported.

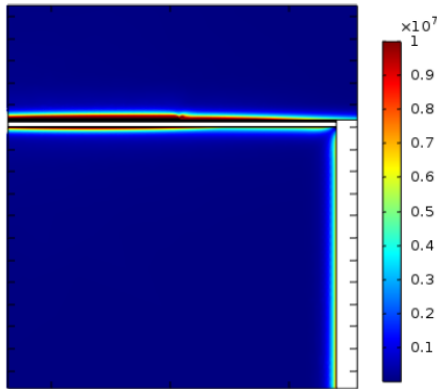


Figure 4: Total thermo-viscous power dissipation density $[W/m^3]$ in the fluid domain, numerically computed by means of COMSOL Multiphysics 5.2. The region in which the losses are concentrated is the so-called boundary layer; in white the solid domain.

The structural Q-factor Q_{struct} , which determines the value of the adopted isotropic structural loss factor

$\eta_{struct} = 1/Q_{struct}$, is calculated subtracting the inverse of Q_{fluid} to the inverse of the measured Q_{tot} , and extracting the inverse of the result (as common in parallel impedance reduction) [11]. The final value is $Q_{struct} = 140$.

Going further, the Sound Pressure Level (SPL) can be computed in every point of the acoustic domain and outside of it by means of the Helmholtz-Kirchhoff integral technique (the so-called *far field* calculation technique). The numerically estimated SPL frequency response at 3.5 cm on the vertical axis of symmetry of the diaphragm is shown in Fig. 5. It is possible to notice that the maximum value occurs in correspondence of the resonance frequency of the membrane and it is associated to a non-directional emitted pressure wave, which is typical of a PMUT device not inserted in a protecting packaging structure. For the operational frequency, the value of the computed SPL is compared with the measured one (red star Fig. 5). The experimental value is obtained setting a microphone, with sensitivity equal to 0.9 mV/Pa, in the same position of the calculated datum. The microphone output voltage and the input voltage provided to the PMUT are shown in Fig. 6.

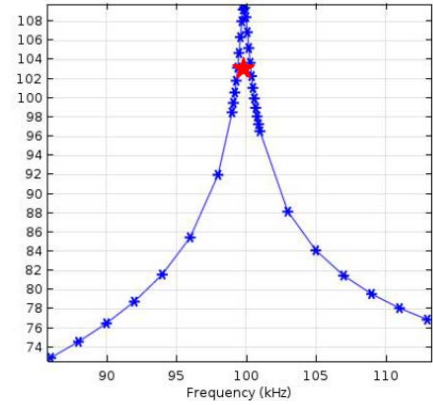


Figure 5: Sound Pressure Level [dB] at 3.5 cm on the vertical axisymmetric axis (blue asterisks). the numerical experimental result is highlighted (red star).

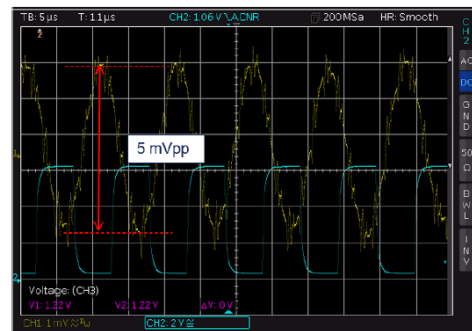


Figure 6: Microphone output voltage in sound intensity measurement (yellow line) at 3.5 cm on the vertical axisymmetric axis, in which is highlighted the 5 mVpp. Input voltage from 0 to 6 V square wave at 100 kHz provided to the PMUT.

The SPL experimental value detected by the microphone is about 103 dB while the numerically predicted one is 109 dB. The over-estimation of the sound intensity by the model is due to the presence of other source of losses not taken into account (e.g. cross-talk among membranes belonging to the same die).

4. Conclusions

In this paper the results obtained with a comprehensive Multiphysics modelling of an air-coupled PMUT are presented, together with their preliminary experimental validations for the mechanical and acoustic responses. In the literature, the most common air-coupled PMUTs are characterized by operational frequency above 200 kHz, while for the presented system the operational frequency is 100 kHz. This difference introduces many challenges due to the non-linearities provided by the high membrane aspect ratio.

The complete simulation of the device's behavior, considering the full multiple coupling among the different physics involved, can guide the designers through the effective control of frequency and quality factor.

To improve the numerical model, further experimental validations in the acoustic domain are in progress (e.g. in order to detect and validate the directivity of the emitted wave the SPL polar diagram must be reconstructed by means of triaxial sound intensity test). Finally, to validate the value of Q_{struct} , it is necessary to perform a harmonic perturbation test over the membrane in a vacuum space.

Furthermore, the adopted axisymmetric modelling is perfectly suited for the simulation of the emission of waves from a circular diaphragm, following the fundamental eigenmode; conversely, to simulate the sensing phase, induced by the echo coming back from an obstacle with a generic geometry, a full 3D model is required.

Acknowledgments

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