Ultrasound Pressure Field Of A Resonating Piezoelectric Membrane With Three Excitation Electrodes.

Vassil Tzanov, Eyglis Ledesma, Francesc Torres, Nuria Barniol
Department of Electronics Engineering, Universitat Autonoma de Barcelona, Spain

The current work shows the possibility for a pressure field simulations in time domain at distances which are an order of magnitude larger than the size of a defined MEMS transducer. The domain of the acoustic media is limited to a specific volume in front of the transducer. The boundaries of this volume have open boundary conditions and a specially designed shape that together diminish the acoustic reflections. Thus, it allows for a 3D simulation of the acoustic field while the necessary computation resources are significantly reduced if compared to a solid hemispherical acoustic domain.

Introduction

Micromachined ultrasound transducers can work as a sensor or actuator for measuring fluid speed and direction, mixing and exciting particles (sonication), taking images (ultrasonography), non-destructive testing and many other purposes in various fields [1]. In this work, a COMSOL 3D-model of a piezoelectric membrane has been built. It consist of a circular AlN-layer in between two top and one bottom Al-electrodes, and a conformal passive SiO_2 top layer, all immersed in a fluid domain where the pressure field propagates; see Fig. 1.

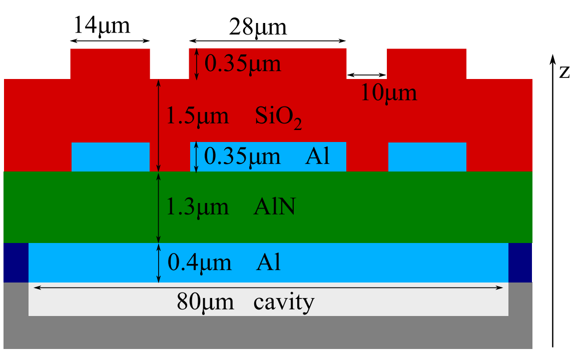

Figure 1: Shematic view of the PMUT layers. From the bottom, substrate layer with a cavity (grey), Al-bottom and top electrodes (blue), AlN-piezoelectric layer (green), conformal top $Si0_2$-passive layer (red).

The proposed models use multi-physics coupling between Acoustics, Solid Mechanics and Electrostatics [2]. Three studies were performed and compared with experimental results. Firstly, an "Eigenvalue Study" computes the resonance frequencies of the device. A "Frequency Domain Study" is used for the detection of the fundamental resonance peak at different acoustic medias, namely air and Fluorinert (FC-70). Finally, a "Time-domain Study" represents the modelling of the experimental setup in our lab where several voltage pulses are applied to the electrodes and a hydrophone is measuring the acoustic signal at 3.8mm from the transducer. By using a non-trivial domain with a spherical radiation boundary conditions we have computed the pressure up to 4mm away from the device. We have been working with three different actuation strategies. More precisely, the transducer was excited by its inner or outer top electrode, or differentially where both top electrodes have anti-phase signals. The simulated medium in the time domain is Fluorinert.

Theory and experimental set-up

If the pressure at a particular point away from the transducer (not in the near field) is known, we can extrapolate the absolute value of the pressure for further distances by using the equations below; see [1, 3].

$$p_{ff} = p_0 R_0 / s \quad \text{, where} \tag{1}$$

$$p_0 = \rho_{aco} c_{aco} u_{avg} \ \text{ and } \ R_0 = A/\lambda \tag{2}$$

p_{ff}- far-field pressure
s- distance to the membrane along the z-axis
ρ_{aco}- density of the acoustic media
c_{aco}- speed of sound in the acoustic media
u_{avg}- average velocity of the membrane
R_0- Rayleigh distance
A- surface area of the membrane
λ- wavelength of the pressure wave

The exact displacement of the PMUT in air and Fluorinert have been measured at Polytec, Germany by using a Laser Doppler Vibrometer (MSA-500, Polytec). The measured modes and the normalised displacement with all electrode actuation configurations are shown in Tables 1 and 2 respectively. Also, the quality factor for the mode (0,1) in Fluorinert and in Air have been measured to be Q_{Air} = 222.7 and $Q_{Fluorinert}$=2.6.

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media (mode)	Air (0,1)	Air (1,1)	Air (2,1)	Air (0,2)	Fluorinert (0,1)
modes [MHz] experiment	5.64	11.3	18.06	20.34	2.2
modes [MHz] simulation	5.57	11.28	18.6	20.87	2.08

Table 1

The acoustics set-up consist of a container with Fluorinert where the PMUT is situated at the bottom. Above the PMUT, at a distance of 3.8mm a hydrophone immersed in the fluid measures the resulted pressure field; for detailed explanation of the set up see [4]. The PMUT is actuated by different electrode configurations where 6-cycles of 10V peak-to-peak sinusoidal signal is applied. The three electrodes allow for excitation due to capacitive force between the inner top electrode (AC signal) and the bottom electrode (grounded), between the outer top electrode (AC signal) and the bottom electrode (grounded), and a differential excitation where both top electrodes have anti-phase AC signal and the bottom electrode is grounded.

Simulations and comparison with the measurements

Geometry, materials and boundary conditions

The geometry of the PMUT device consist of several cylinders that represent the different material layers where the substrate layer and the cavity (see Fig. 1) are not simulated. The cylinder that represents the bottom electrode is divided by two. An inner part (cylinder) and an outer part (hollow cylinder) denoted in Figure 1 by light and dark blue, respectively. The inner part is the one above the cavity which defines the diameter of 80μm of the resonating circular membrane. The outer part has its bottom annular boundary defined in COMSOL as Fixed Constraint, hence the PMUT membrane is clamped at its circular boundary. The AlN-piezoelectric layer is a cylinder (green) while the top Al-electrodes (blue) are an inner cylinder and an outer hollow cylinder. The diameter of the inner electrode is 28μm and the gap to the outer electrode is 10μm. The diameter of the outer electrode is 76μm. Both top electrodes are covered by a conformal passive layer of SiO_2 (red). The resulted geometry of the passive layer is achieved by boolean operations of cylinders.

The acoustic domains are solid hemispheres for the Eigenvalue and the Frequency domain simulations, and series of overlapped solid hemispheres for the Time domain simulation. Thus, the different volumes and acoustic medias led to 3 models that consist of different studies. One for the Eigenvalue and the Frequency domain in Air and another for the Frequency domain simulation in Fluorinert. The third one is the Time domain simulation in Fluorinert. In the first two models the acoustic volume is a solid hemisphere with lower boundary that consist of Acoustic-Structure Boundary and a Sound Hard Boundary. The rest has Spherical Wave Radiation boundary conditions. The third model has an acoustic volume that consist of multiple solid hemispheres. Again, all the boundaries of the acoustic domain except the Acoustic-Structure and the Sound Hard Boundaries have Spherical Wave Radiation boundary conditions. See the Physics subsection for more details on the boundaries.

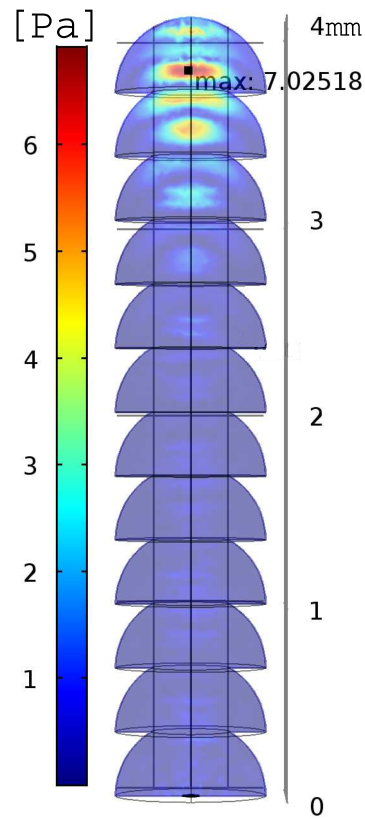

Figure 2: Pressure field in Fluorinert computed at 8.6μs where the maximum pressure of 7Pa appears near 3.8mm.

When the multiple hemispherical domains overlap, they form a long corridor of acoustic media in front of the transducer. We will call aperture the width of the corridor where one hemisphere intersects with another. It can be controlled by the radii of the hemispherical domains and by how much they overlap. Comparing to the single hemispherical domain, the overall volume of the media where the pressure field has to be computed

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is drastically decreased, hence the amount of computational power is decreased too. Therefore, our acoustic domain allows a simulation that computes the pressure up to 4mm where 12 hemispheres with radius 395μm overlap 15% of their radii; see Figure 2. The resulted aperture is 416.16μm for the 15%- and 344.35μm for the 5%-overlapping.

In order to keep the reflections as low as possible the shape of the acoustic media has to be such that the angle of incidence of the wavefront with the boundary of the acoustic domain must be as close to 0 as possible [5]. Thus, the bigger apertures (bigger percentage of overlapping or radii) will result in bigger angle of incidence with the succeeding hemisphere, hence, more reflections. Otherwise, smaller apertures will result in greater absorption of the pressure field while propagating because a larger portion of the wavefront will hit the spherical radiation boundaries. This idea led us to the solid multiple hemispherical domain presented here, see Figures 2 and 3.

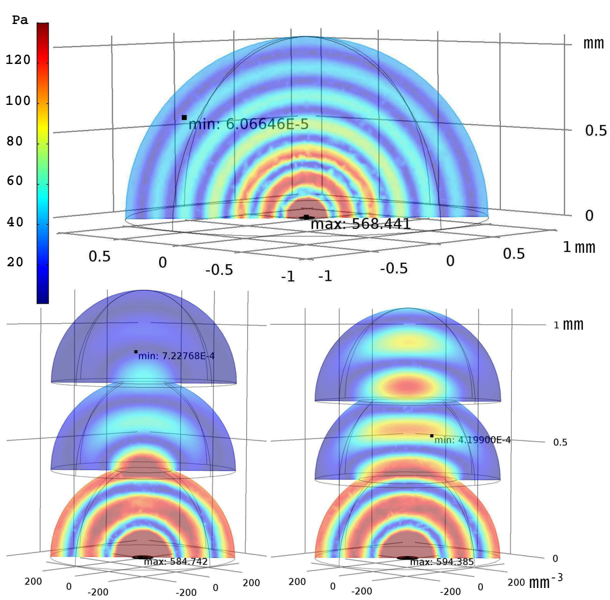

Figure 3: Comparison between the different pressure fields in Fluorinert resulted from single-sphere computation and three-sphere computations with 5% and 15% overlapping of their radii.

Mesh

The PMUT device is much narrower in Z-direction than in X- and Y-directions and a swipe meshing along Z-axis is preferable; see Fig. 1. Yet, cylinders of different diameters are necessary for the PMUT's geometry that makes a swipe meshing very hard to achieve for all its components. Thus, the meshing process starts with Free Tetrahedral triangulation of the *AlN*-layer where the minimum and maixmum element sizes are 1μm and 5.2μm, respectively. Then, Swipe meshing is performed downwards for the bottom *Al*-layer and upwards for the *Al*- and SiO_2-layers except the top 0.35μm of the SiO_2. This volume of the passive layer that resembles the shape of the top electrode has Free Tetrahedral meshing with minimum and maximum element sizes of 1.5μm and 20μm, respectively. The tetrahedral triangulation of the top 0.35μm of the PMUT is necessery because it is surrounded with the hemispherical acoustic media domain which is also free tetrahedral. The maximum diameter of the tetrahedral element of the acoustic media is prescribed by the speed of sound in air and Fluorinert which are 343 and 689m/s respectively, see [2, 3].

Physics

The Physics used are Solid Mechanics, Electrostatics, Pressure Acoustics (frequency and time domains) and Multiphysics. The Solid Mechanics has Linear Elastic Materials and Piezoelectric material nodes where damping is defined in the Linear Elastic Materials nodes by using Isotropic Loss Factor option. In our simulation the loss factors of *Al*- and SiO_2-layers have the ratio 3:2. The damping of the Piezoelectric material is defined by its elasticity matrix which is given as a material property. As mentioned above, a Fixed Constrains node defines part of the lower boundary of the bottom *Al* electrode as fixed prescribing the boundary conditions of the membrane.

The Electrostatics has two Terminal and a Ground nodes that correspond to the two top and one bottom *Al*-electrodes. The voltage in the Electrostatics and the Pressure Acoustics (frequency domain) that is set in the Terminal nodes is fixed. In the time domain Pressure Acoustics the voltage defines 6 pulses in phase with the frequency of the fundamental mode of the membrane in Fluorinert. Thus, in our simulations $V_{dc} = 16.7/2$V and $V_{ac} = V_{dc}\sin(2\pi ft)(t <= cycles/f)$, where $cycles = 6$ and $f = 2.08e+6$Hz. For the both domains the terminal voltage has to be set so the specific excitation strategy is specified, more precisely, using only the inner, only the outer or both electrodes. For the differential excitation the voltage of Terminal 2 is specified by using the COMSOL function $-es.term1.V0$.

In the Pressure Acoustics (frequency and time domains), the open boundary conditions are set to Spherical Wave Radiation for all the sides of the hemispheres except the one in the plane of the transducer. This, boundary is prescribed in the Multiphysics.

The Multiphysics has two nodes, Piezoelectric effect and Acoustic-Structure Boundary. In the Piezoelectric effect the Solid Mechanics and Electrostatics are coupled. In the Acoustic-Structure Boundary the Solid Mechanics is coupled with the Pressure Acoustics. Also, in this node we define the boundary that transmits the oscillations in between the device and the acoustic media. In our case this is the upper boundary of the passive layer of the device.

Solver settings

There are three solvers involved in the current work Eigenfrequency, Frequency Domain and Time Dependent. All of them are defined in different studies, thus we have three studies. The Eigenfrequency solver includes only Solid Mechanics where the geometric nonlinearity option is included. The Eigenfrequency solver searches for 6 eigenfrequencies around 0.

Frequency Domain solver uses all physics interfaces except the time dependent pressure acoustic (if included in the file). An initial range of frequencies was specified and after few simulations the time-step was decreased down to 0.002MHz.

The Time Dependent study computes in the range from 0 to 10μs in time intervals of 0.02μs. The geometric nonlinearity option is selected.

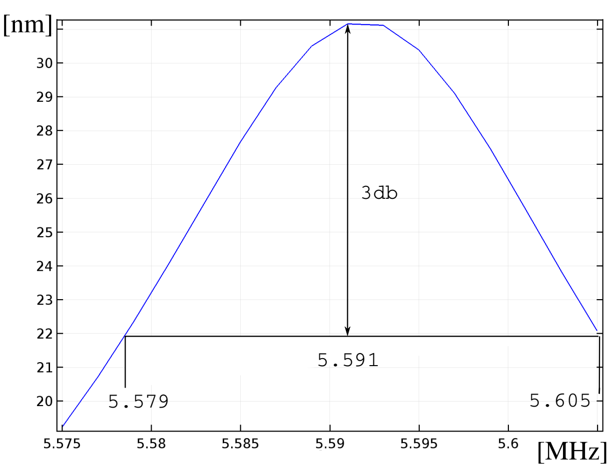

Figure 4: Displacement versus frequency plot resulted from the Frequency domain study which is used for the calibration of the model with the experiment.

Results

The results from the Eigenfrequency study in Air can be seen in Table 1 where they are compared with the measured values. The following is a Frequency Domain Study where the resonance peak in Air has been searched near the fundamental mode of 5.64 MHz. Once the peak was found at 5.591MHz, the loss factors of Al and SiO_2 were varied so the displacement amplitude of the membrane fits with the measurements. Therefore, for Al-loss factor equal to 0.006 and SiO_2-loss factor equal to 0.004, at voltage of 8.35V$_{pp}$ (internal el. excitation), the resulted displacement amplitude at the center of the membrane was 31nm; see Fig. 4. In comparison, the displacement amplitude measured at Polytec is 30.94nm at 8.31V$_{pp}$ applied. Also, the Q$_{Air}$ from the simulation and the measurements are 215.04 and 222.7, respectively.

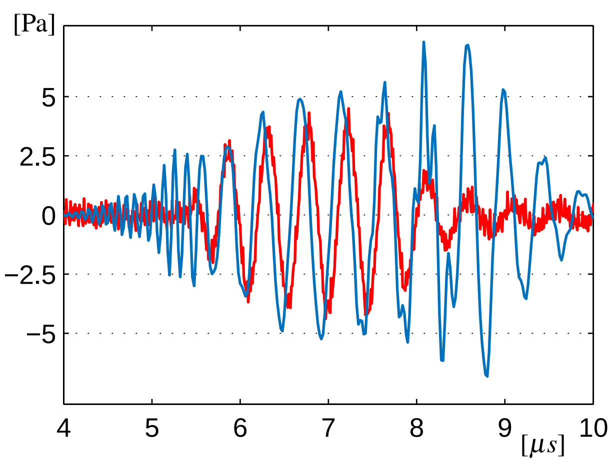

Figure 5: Comparison between the experimental (red) and simulated (blue) wave-trains of the pressure field at 4mm in Fluorinert. The excitation is achieved by the internal electrode.

Once the model is calibrated, the media is changed to Fluorinert (FC-70). In Fluorinert the frequency peak appears at 2.08MHz (see Table 1) and the comparison of the measured and simulated displacements can be seen in Table 2. The Q$_{Fluorinert}$ from the simulation and the measurements are 2.97 and 2.6, respectively.

The acoustic measurements were only in Fluorinert and the Time domain study is computed only in this acoustic media. The displacements resulted from the frequency domain studies and from the time domain studies are almost identical.

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	Pressure$_{pp}$ at 3.8mm in/out/differential	Displacement$_{pp}$ of the membrane in/out/differential
Experiment	0.8/2.7/4 Pa/V$_{pp}$	0.1/0.29/0.38 nm/V$_{pp}$
Frequency domain		0.07/0.12/0.18 nm/V$_{pp}$
Time domain	0.84/1.57/2.46 Pa/V$_{pp}$	0.07/0.12/0.18 nm/V$_{pp}$

Table 2

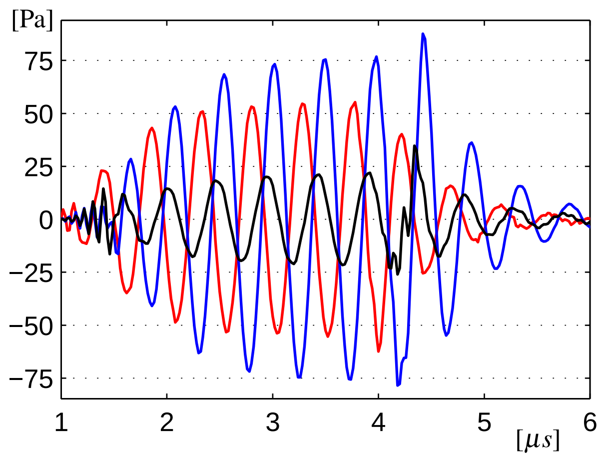

Figure 6: Comparison between the simulated wave-trains of the pressure field at 1mm. 3 hemispheres with radius of 395μm which radii overlap 15% (blue), 3 hemispheres with radius of 395μm which radii overlap 5% (black) and a single hemisphere with radius of 1mm (red). The excitation is achieved by the internal electrode.

The computation of the pressure in Fluorinert at a distance of 1mm by using hemispherical media domain with radius of 1055μm takes 2h:58min. In comparison, if computed by using 3 hemispheres with radius of 395μm which radii overlap 15% it takes 52min. For a single hemispherical domain, when the radius is increased to 3mm the simulation demands more than 32GB of RAM which is the limit of our computer. While, by using 12 hemispheres, 395μm radius and 15% overlaped, our simulation computes the pressure up to 4mm and finishes in 1h and 47min. In Figure 5, the comparison between the measured and the simulated pressures at 4mm is shown.

It should be noted that the quality of the resulted pressure field is not as high as if computed in a single hemispherical domain. In Figure 3 we can compare the wavefronts produced by an identical transducer excited by the inner electrodes with 8.35V$_{pp}$ where all three simulations are stopped at 3.4μs. If we compare the fourth wavefront (0.5mm away from the membrane), the domain with aperture that corresponds to 5% overlapping results in approximately 55Pa in the middle of the wavefront which is lower than in the other simulations. Oppositely, in the middle of the same wavefront, the domain that corresponds to 15% overlapping has more than 100Pa while the single hemispherical domain results in approximately 80Pa. Moreover, the wavefronts of the single hemispherical domain appear a bit closer to the transducer which can be confirmed in Fig. 6. Figure 6 compares three wave-trains from the same simulations presented in Fig. 3, at a distance of 1mm from the membrane. Here it must be pointed out that the pulses in the single hemispherical domain (red) start decreasing after the sixth peak which is consistent with the six electrical pulses form the inner electrode. Curiously, the other two simulations have an additional 7th pulse before the decrease of the oscillation. Moreover, this 7th pulse shifts the wavelength of the wave-packet, especially in the case of 5% overlapping domain. This unwanted effect gets more obvious at lager distances from the acoustic source, see Fig. 5. Finally, in Figure 7 we compare the decrease of the maximum pressure with the distance when computed in single and multiple hemispherical domains. The blue curve is the computed pressure field in multiple hemispherical domain with 15% overlapping. On the top of it, the black and the red curves correspond to the computed pressure field in single hemisphere up to 1mm and the extrapolated far-field pressure up to 4mm; see Equation (1). The figure shows that we can expect better results from the multiple hemispherical domain at distances greater than 2mm.

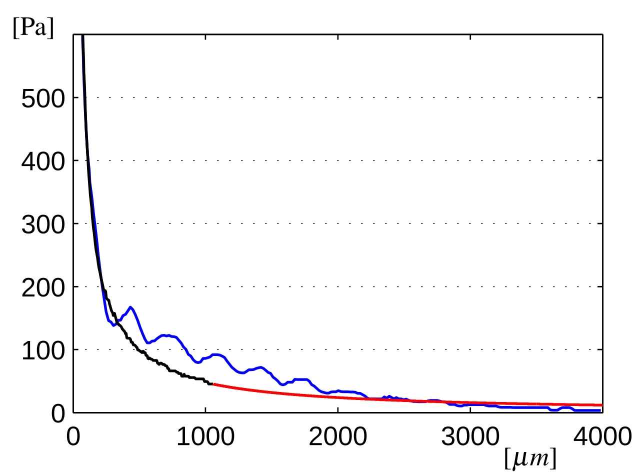

Figure 7: Comparison between the single-sphere simulation (black), the extrapolation from it (red) and multiple-sphere simulation (blue).

Conclusion

Our models allow different geometries and materials to be investigated and are well calibrated to fit with the conducted measurements. We predicted the resonant frequency of the device in air and Fluorinert, the Q factors of the device in different media as well as the most efficient excitation strategy. Also, by using specially designed boundaries we reduced the needed computational resources for the time-domain simulation of the pressure field. Still in a good agreement with the experiment at 3.8mm. The models have the ability to compare electrode designs, layers' thicknesses and layers' materials when aiming at an optimal ultrasound actuating performance.

Acknowledgement

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