A REPORT

ON

DESIGN AND INVESTIGATION OF PHOTOACOUSTIC DETECTOR

BY

Reva Teotia 2019A3PS0268P

AT

CSIR-CEERI, Pilani

A Practice School-I Station of

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI

(June-July, 2021)

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Prepared in partial fulfillment of the
Practice School-I Course Nos.
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Key Words: microelectromechanical systems (MEMS); acoustic sensors; photoacoustics; diaphragm displacement; mechanical sensitivity;

Project Areas: Design of MEMS microphone; Photoacoustic detector for gas-sensing

Abstract: Advancements in microelectromechanical system (MEMS) technology over the last several decades have been a driving force behind miniaturizing and improving sensor designs. This project aims the design a MEMS microphone as a photoacoustic detector for gas sensing applications. The work includes the theoretical background of photoacoustic spectroscopy and the setup for gas sensing applications. The design and performance optimization techniques of a microelectromechanical (MEMS) condenser microphone are studied and described using several established plate theories and numerical analysis. COMSOL Multiphysics 5.6 is used to perform analysis of the various microphone parameters on the performance of the MEMS microphone.

Signature of Student
Date - 20/07/2021

Signature of PS Faculty
Date - 20/07/2021

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1.Introduction

The photoacoustic effect was first reported by A. Bell (1880), he found that thin disk generated sound waves when exposed to a rapidly interrupted beam of sunlight; in the following years, several renowned scientists studied this new phenomenon. With the advancement in technology, photoacoustic spectroscopy-based gas detectors are capable of ultra-sensitive spectroscopic examination. Photoacoustic spectroscopy is one of the most exciting areas of research in physics and chemistry, covering a broad range of applications from agricultural to biological, including atmospheric monitoring, space science, and air-quality measurements to security and workplace surveillance, in addition to its great potential in preclinical and clinical biomedical applications. As microfabrication technology has made a rapid growth over the past decade, the gas detectors are also getting smaller in size. It has made possible the incorporation of sensors in personal and wearable devices. This will make personal health monitoring devices readily available for the general public.

The objective of this project is to design a MEMS Microphone as photoacoustic detection for photoacoustic spectroscopy based gas sensing applications. The report begins with the theoretical background of photoacoustic spectroscopy and then goes into the working principle, specifications and design aspects of the MEMS microphone. The study mainly focuses on capacitive MEMS microphones and compares the various methods that researchers have used to improve the sensitivity of the MEMS microphone. The theoretical equations for microphone parameters are then presented. COMSOL Multiphysics software has been used to perform various studies and comparisons for improving the open-circuit sensitivity of the microphone. The work also includes simulation of circular corrugated diaphragm and compare the effect of residual stress on the mechanical sensitivity.

2. Photoacoustic spectroscopy

2.1. Working principle

Photoacoustic spectroscopy is based on the photoacoustic effect. The photoacoustic effect is the formation of sound waves following light absorption in a material sample. The laser is tuned to a suitable absorption line and modulated at a fixed frequency in the audio range.
The PA effect in gases can be divided into five main steps

I. Modulation of the laser radiation (either in amplitude or frequency) at a wavelength that overlaps with a spectral feature of the target species.
II. Excitation of the target molecule by absorption of the incident laser radiation.
III. Energy exchange processes: the energy which is absorbed is almost completely converted to the kinetic energy of the gas molecules, the kinetic energy, and then converted into periodic local heating at the modulation frequency.
IV. Expansion and contraction of the gas in a closed volume gives rise to pressure variation which is an acoustic wave.
V. Detection of the resulting acoustic waves with microphones.

The PA signal measured by the microphone is given by:

$$S = C.P(\lambda).\alpha(\lambda)$$

where C is the cell constant in the unit of Vcm/W,
P the optical power of the laser source and
α the absorption coefficient which is related to the gas concentration (N, number density of molecules) and absorption cross-section (σ) by $\alpha = N\sigma$.
The cell constant depends on the geometry of the sample cell, the beam profile, the microphone response, and the nature of the acoustic mode.

A photoacoustic spectrum is recorded by tuning the coupled light source to different wavelengths and measuring the pressure changes in the cell. Via this spectrum, the absorbing compound of the sample can be identified.

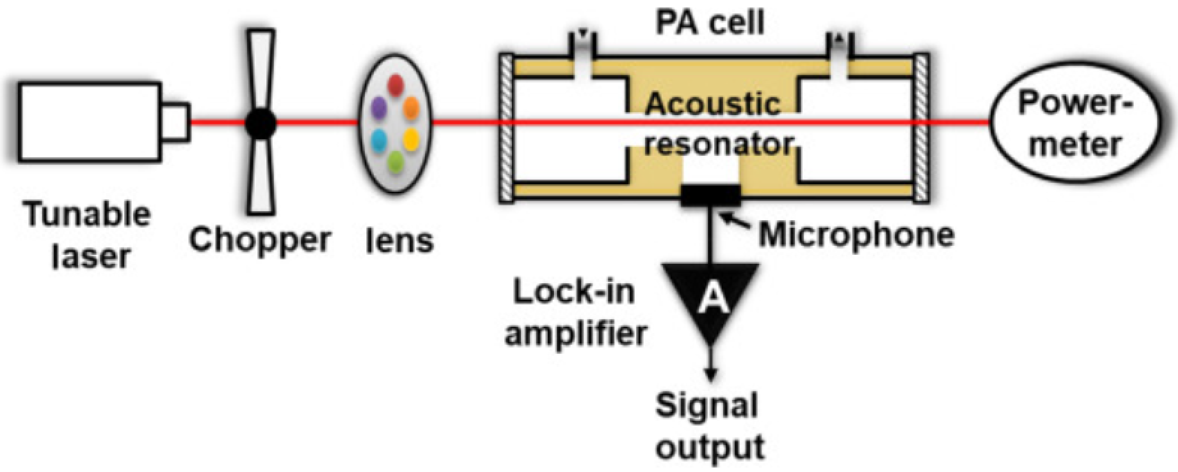


Figure 1: representation of the setup for photoacoustic spectrometer

2.2. Radiation sources

To optimize the photoacoustic signal and enable specific detection of a gas species, the use of laser sources plays a pivotal role in most laboratory setups. The high spectral density and beam quality allows for the design of ultra-sensitive devices and the use of enhancement strategies to increase the acoustic signal allows for the building of highly sensitive and specific analyzers. Depending on the requirements of a specific measurement task, LEDs or thermal light sources might prove more suitable and in fact, many commercially available solutions use simple photoacoustic setups.

2.3. Detectors

As mentioned above the acoustic disturbances generated in the sample are detected by some kind of pressure sensor. These include designs based on gas-filled or unfilled MEMS microphones, optical microphones based on Fabry–Pérot interferometers (FPIs), or quartz tuning forks (QTFs). Sensors based on FPIs or QTFs feature higher sensitivities. However, these also require more expensive light sources and have larger form factors. Photoacoustic sensors, using highly sensitive MEMS microphones, have emerged as compact, low-cost sensors with high sensitivity and stable operation.

3. MEMS Microphone

MEMS technology has revolutionized this industry by developing ultra-small-size, lightweight, low-power, low-cost, and compact-size devices. MEMS microphones have higher performance density, can be reflow soldered, and have less variation in sensitivity over temperatures. MEMS microphones can be easily integrated with other microlevel circuitry, which makes it perfect for various applications, including but not limited to smartphones and tablets, as well as automotive, industrial, and medical applications. Also, the reduced size of MEMS microphones makes it perfect for use in the form of arrays of multiple microphones for different applications in small products. The conversion of sound pressure waves into electrical signals is performed by different transduction mechanisms, i.e., piezoelectric, piezoresistive, optical, and capacitive. Two of them are discussed below.

3.1. Piezoelectric Microphones

Piezoelectric is one of the transduction mechanisms used to sense the motion of the flexible membrane of a microphone. A piezoelectric material attached to the microphone membrane gets stressed due to the membrane's movement from sound waves, which generates an electrical voltage as an output called a piezoelectric effect

The commonly used piezoelectric materials are zinc oxide (ZnO), aluminum nitride (AlN), and lead zirconium titanate (PZT). Both ZnO and AlN are non-ferroelectric materials while PZT is a ferroelectric material. ZnO has better availability and less demanding vacuum conditions, while AlN has compatibility with CMOS processing and has a higher resistivity than ZnO. The piezoelectric coefficients of PZT are higher than the other.

A piezoelectric microphone diaphragm can be formed by sandwiching the piezoelectric material between two metals. Diaphragms of piezoelectric microphones can be circular or square and cantilever or double cantilever. Cantilever-based diaphragms are free from residual stresses as compared to clamped-clamped diaphragms. Circular diaphragms show higher sensitivities as the maximum stress distribution in the circular diaphragm is uniform along the circumference as compared to that in the square diaphragm in which the maximum stress distribution is along a part of the edges

Vesper has produced commercially available piezoelectric microphones for smartphones, wearable technology, and IOT. The product VM1000 with a package size of 3 76 mm × 2 95 mm × 1 1 mm has a sensitivity of -38 dBV, SNR of 62 dBA (for 20 Hz to 20 kHz bandwidth), and 64 dBA (for 20 Hz to 8 kHz bandwidth), and a maximum pressure of 125 dBSPL. This was further improved to 135dBSPL of AOP. Figure 2 shows the simplified structural view of Vesper's VM1000 piezoelectric microphone. Some other market players are Bosh, Analog Devices, Infineon, and Knowles.

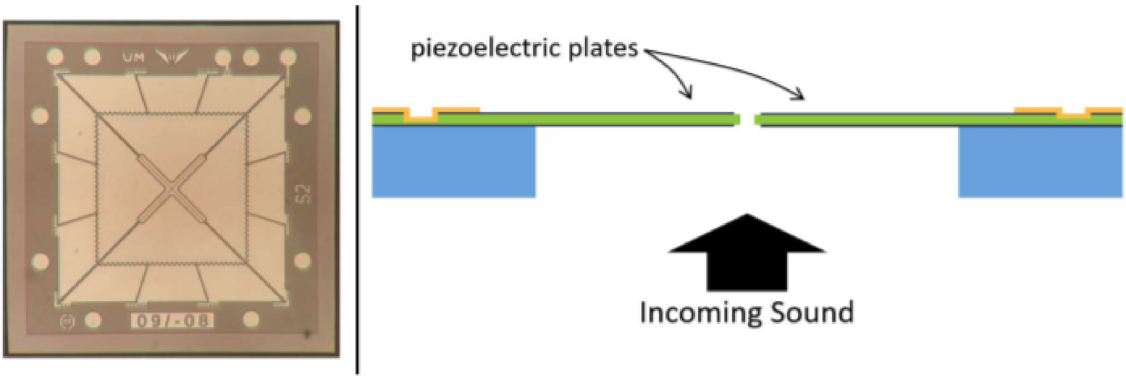


Figure 2: Top-view (left) & cross-sectional drawing (right) of Vesper piezoelectric MEMS microphone VM1000 (source: Vesper Technologies Inc).

3.2. Capacitive Microphones

A capacitive microphone contains a backplate and a flexible membrane fabricated on a silicon wafer. The perforated backplate allows the sound pressure wave to enter, which causes the flexible membrane to move. The movement of the flexible membrane causes a capacitance variation between the membrane and a fixed plate, which is converted into an electrical signal through various types of interface circuitry.

The major components of a capacitive microphone are the movable acoustic diaphragm and fixed backplate. Both are separated by an air gap, and an insulator was used as the spacer. The backplate consists of acoustic holes because the squeezed air between the diaphragm and the backplate becomes a mechanical damper and reduces the ability of the diaphragm to vibrate, especially at high frequency.

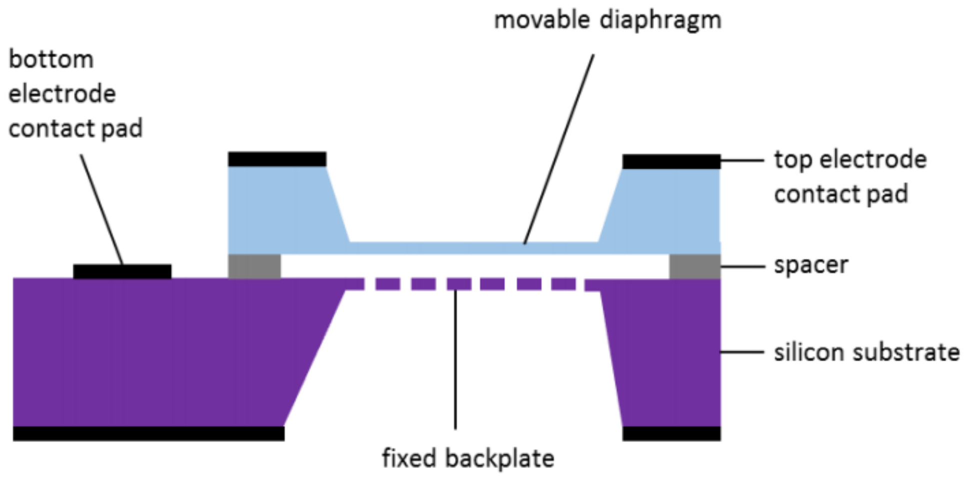


Figure 3: Basic structure of MEMS capacitive microphone

The acoustic diaphragm can be made of Si, poly-Si, Si_3N_4, or Al. The diaphragm has to be patterned to control residual stress. Compared to the square flat diaphragm, the corrugated circular diaphragm gives higher open-circuit sensitivity and larger corrugation depth leads to higher sensitivity. Several research groups have used springs and slits in the diaphragm to reduce stress.

The backplate is the second most important component as it plays an important role in determining the capacitance by fixing the amount of charge. Si and poly-Si are mostly used as backplate material. When the acoustic diaphragm vibrates, the air between the diaphragm and the backplate acts as a damper and reduces the sensitivity. Research groups have found that air gap is inversely proportional to the sensitivity and that at least 10 μm of air gap is required to achieve stable operating microphone, achieving 10 mV/Pa of sensitivity.

Current MEMS microphones can be found in the range of about 55 dB to 70 dB SNR. Currently, Infineon Technologies has a high-performance microphone with the highest SNR of 69 dB with an acoustic overload point (AOP) of 130 dBSP. Bosch has designed a microphone with a spring attached circular diaphragm. The membrane is made up of polysilicon with 0.6 mm in diameter. The total chip size of the microphone is 1 mm2. The frequency response of this microphone was found to be 12 kHz, and the SNR was calculated as 58 dB. Analog Devices, Knowles Electronics, STMicroelectronics, and Akustica are some of the key manufacturers of capacitive MEMS microphones.

3.3. Microphone specifications

In cases of pulsed PA spectroscopy the selection of the microphone is particularly crucial. It is actually impossible to select a microphone that is optimized for any PA measurement. In practice, it is necessary to select from the most significant microphone characteristics, such as responsivity, dynamic range, and frequency dependence, those that are most relevant for the specific PA measurement. For trace gas sensing applications, microphones with high responsivity and SNR but small bandwidth of ~20 kHz are employed. Most commercially available microphones have the bandwidth in the audible range which makes them feasible for the photoacoustics based trace gas sensing applications. The currently used commercial microphone which is employed in CO_2 detection by Infineon has SNR of 69dB(A). To get a better understanding, the general microphone specifications are explained in this section.

3.3.1. Sensitivity

The sensitivity of a microphone is the electrical response at its output to a given standard acoustic input. The standard reference input signal for micro-phone sensitivity measurements is a 1 kHz sine wave at 94 dB sound pressure level (SPL), or 1 Pa. Microphone sensitivity in decibels (dB) is typically a negative number; therefore, a higher sensitivity is a smaller absolute value.

$$Sensitivity_{dBV} = 20 \times log\left(\frac{Sensitivity_{mV/Pa}}{Output_{REF}}\right)$$

where $Output_{REF}$ is the 1 V/Pa (1000 mV/Pa) reference output ratio.

3.3.2. Signal-to-Noise Ratio (SNR)

The signal-to-noise ratio (SNR) specifies the ratio of a reference signal to the noise level of the microphone output. The SNR is the difference in decibels between the noise level and a standard 1 kHz, 94 dB SPL reference signal. SNR is calculated by measuring the noise output of the microphone in a quiet, anechoic environment. This specification is typically presented over a 20 kHz bandwidth as an A-weighted value (dBA), which means that it includes a correction factor that corresponds to the human ear’s sensitivity to sound at different frequencies.

3.3.3. Dynamic range

The dynamic range of a microphone is a measure of the difference between the loudest and quietest SPLs to which the microphone responds linearly. The dynamic range of a MEMS microphone is the difference between its acoustic overload point (AOP) and equivalent input noise (EIN).

3.3.4. Frequency response

The frequency response of a microphone describes its output level across the frequency spectrum. The high and low-frequency limits are described as the points at which the microphone response is 3 dB below the reference output level at 1 kHz. The reference level at 1 kHz is customarily normalized to 0 dB.

3.3.5. Total Harmonic Distortion (TDH)

Total harmonic distortion (THD) is a measurement of the level of distortion on the output signal for a given pure tone input signal. This measurement is presented as a percentage. This percentage is the ratio of the sum of the powers of all harmonic frequencies above the fundamental frequency to the power of the tone at the fundamental frequency.

$$TDH = \frac{\sum_{x=1}^{5} Power(f_{harmonic\ x})}{Power(f_{fundamental})}$$

A higher THD measurement indicates a higher level of harmonics present at the output of the microphone.

3.3.6. Acoustic Overload Point (AOP)

The acoustic overload point is the sound pressure level (SPL) at which the THD of the microphone's output equals 10%. This is also commonly referred to as the microphone's clipping point. SPLs higher than this specification cause severe nonlinear distortion of the output signal.

4. Theoretical Model of Microphone Parameters

4.1. Open-circuit sensitivity and bias voltage

The open-circuit sensitivity of MEMS microphone is given by the following equation:

$$S = S_e \times S_m = \frac{V_b}{y} \times \frac{\Delta y}{\Delta P}$$

where S_e and S_m are electrical and mechanical sensitivity, respectively, while V_b, y, Δy, and ΔP are bias voltage, air gap, change in the air gap, and change in pressure, respectively.

The bias voltage is applied to the membrane to operate the capacitive microphone. While the bias voltage is directly proportional to the sensitivity, increasing beyond a certain threshold, pull-in voltage, causes the membrane to collapse to the backplate. The pull-in voltage can be represented by the following:

$$V_{PI} = \sqrt{\frac{8ky_o^3}{27\varepsilon A}}$$

where $k = 8\pi\sigma_0 h$ is the effective spring constant of the diaphragm, y_o is the air gap at bias voltage of zero, ε is the permittivity of air, and A is the effective area of the backplate.

4.2. Mechanical Sensitivity of circular flat diaphragm

The center deflection (y) of a flat circular diaphragm with clamped edges and without residual stress, due to a homogeneous pressure (P) can be calculated from:

$$\frac{PR^4}{Eh^4} = \left(\frac{5.33}{1-v^2} + \frac{4\sigma_0 R^2}{Eh^2}\right)\frac{y}{h} + \frac{2.83}{1-v^2}\left(\frac{y}{h}\right)^3$$

where E,σ_0,v, R and h are Young's modulus, residual stress, Poisson's ratio, radius and thickness of diaphragm, respectively.

For small deflection, the mechanical sensitivity of a flat circular diaphragm ($S_m = dy/dP$), by neglecting the 3rd order term, can be expressed as:

$$S_m = \frac{R^2}{4h[\sigma_0 + \frac{4Eh^2}{3(1-v^2)R^2}]}$$

Equation shows that mechanical sensitivity is inversely proportional to residual stress, which depends on fabrication process.

Making shallow corrugations in the diaphragm reduce the effect of residual stress and subsequently increase the mechanical sensitivity.
The corrugated diaphragm with residual stress, σ_0 , acts similar to planar diaphragm with a reduced stress, σ . It means that the stress of a corrugated diaphragm can be written as:

$$\sigma = \eta\sigma_0 \quad \eta < 1$$

where σ is equilibrium stress of corrugation diaphragm, σ_0 is residual stress and η is attenuation coefficient of stress.

4.3. Mechanical Sensitivity of circular corrugated diaphragm

The center deflection of a corrugated circular diaphragm with clamped edges can be expressed as:

$$P = [a_p E\frac{h^4}{R^4} + \frac{4h^2\sigma}{R^2}]\frac{y}{h} + b_p\frac{E}{(1-v^2)}.\frac{h^4}{R^4}.\frac{y^3}{h^3}$$

where a_p is the dimentionless linear coefficient and b_p is the dimentionless non-linear coefficient.

$$a_p = \frac{2(q+1)(q+3)}{3(1+\frac{v^2}{q^2})}$$

$$b_p = 32\frac{1-v^2}{q^2-9}(\frac{1}{6} + \frac{3-v}{(q-v)(q+3)})$$

where q is corrugated profile factor which is given by:

$$q^2 = \frac{S}{L}(1 + 1.5\frac{H^2}{h^2})$$

For small deflections, the mechanical sensitivity of a corrugated circular diaphragm ($S_m = dy/dP$) can be calculated as:

$$S_m = \frac{R^2}{h[4\eta.\sigma_0 + E.a_p.\frac{h^2}{R^2}]}$$

where S, L, H and h are the spatial period, arc length, depth of corrugations and diaphragm thickness, respectively.

4.4. Resonant Frequency

The resonant frequency limits the upper bandwidth of the microphone. It is given by:

$$f_0 = \frac{1}{2\pi}\left[\frac{\frac{8Eh^3/9(1-v^2)R^2}{9(1-v^2)R^2} + \frac{\kappa^{-1}\pi^2R^2}{18y}}{\frac{\rho h\pi^2R^2}{10}}\right]$$

where E, ν, and ρ are Young's Modulus, Poisson's ratio, and density of material, respectively, κ is compressibility of air, y is air gap between the plates, and h and R are thickness and radius of the diaphragm. The equation shows that the frequency is affected by the material properties and dimensions of the diaphragm. Considering the frequency range of human auditory, which is 20 Hz – 20 KHz, the resonance frequency of microphone should be out of this range.

5. Results and Discussion

Main characteristics of MEMS microphone such as mechanical sensitivity, pull-in voltage, and resonance frequency are important parameters that should be analyzed carefully. The diaphragm plays an important role in the determination of mechanical sensitivity of the microphone. This section includes finite element modeling analysis for the effect parameters like initial stress, diaphragm dimensions, and corrugation.
The analysis is done on a MEMS capacitive microphone with poly-silicon diaphragm of radius 0.5mm and thickness 2μm. Details are provided in Table 1.

Parameter	Value
Diaphragm radius, R	0.5 mm
Diaphragm thickness, h	2 μm
Diaphragm material	poly-silicon
Density, ϱ	2320 kg/m^3
Young's modulus, E	160 GPa
Poisson ratio, ν	0.22
Initial diaphragm stress	120 MPa
Air gap thickness, y_0	1 μm
Corrugation height, h_c	5 μm
Corrugation width, w_c	20 μm
Distance between corrugation, b_c	15μm
Bias Voltage, V_b	9 V

Table 1: Geometry and Material Properties

5.1. Variation of diaphragm radius

The open-circuit sensitivity increases with increasing diaphragm radius, as the capacitance is directly proportional to the area. The simulation results in figure 4(a) shows that an increase of 0.5mm radius can increase the sensitivity up to 20dB. Figure 4(b) shows that the increase in diaphragm radius increases the displacement of the center of the membrane.

With the increase in radius, the displacement increases but this, in turn, reduces the natural frequency. This leads to reduced bandwidth of the microphone. Also, the goal of MEMS is to reduce the size of the device and therefore we don't want microphones with large diaphragm radius.

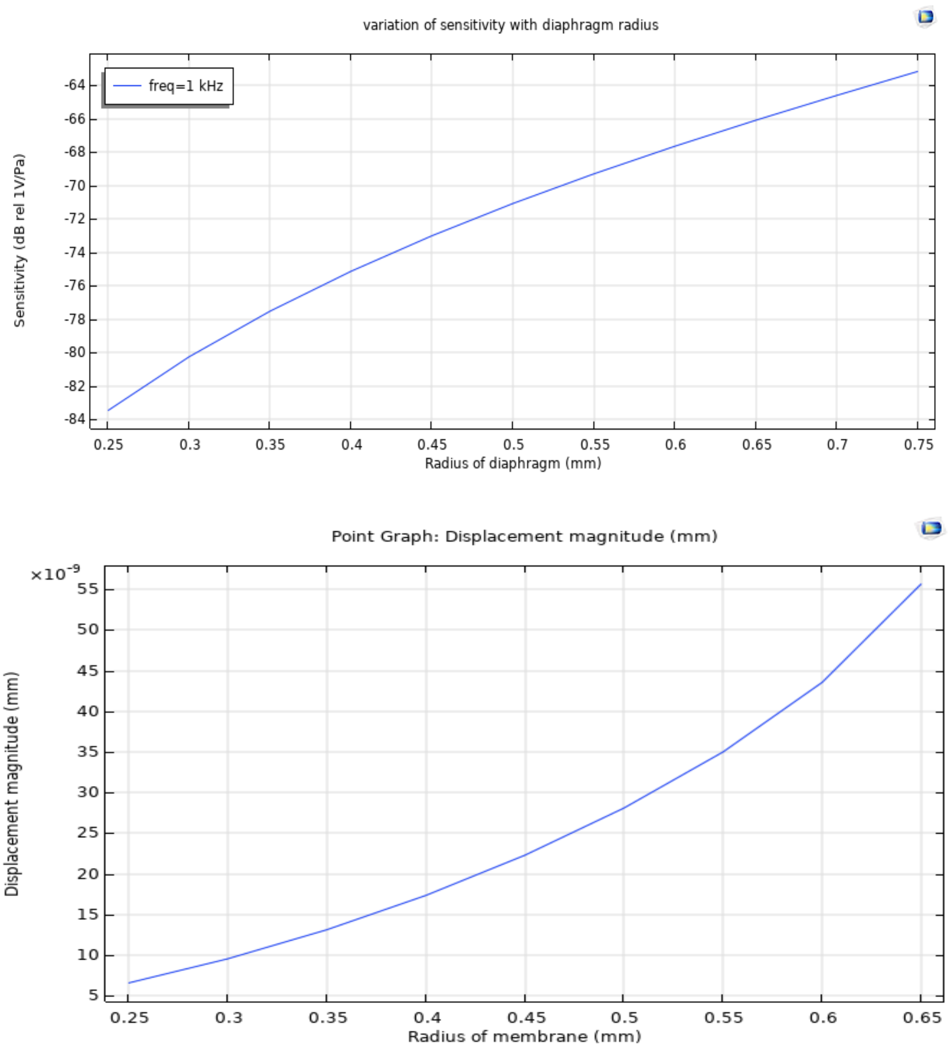


Figure 4(a) and 4(b): Variation of Sensitivity and displacement of the center of membrane respectively, with increasing membrane radius

5.2. Variation of bias voltage

The displacement of the center of the diaphragm increases with increasing voltage. With increasing bias voltage from 1 V to 9 V, the sensitivity increased from -77.7 dB to -57.4 dB. The voltage cannot be increased beyond a threshold, pull-in voltage, because the diaphragm then collapses with the backplate. The calculated value of pull-in voltage for the simulated model is 16V, which matches the simulation result.

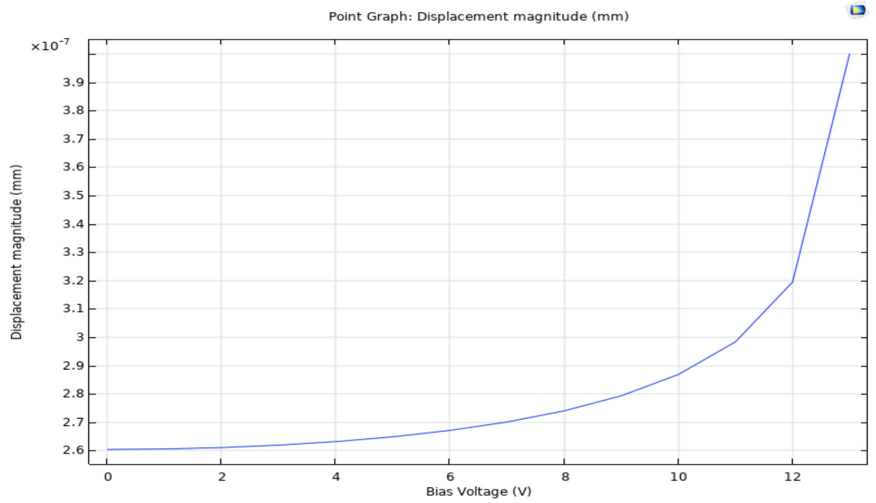


Figure 5(a): Center displacement with varying voltage

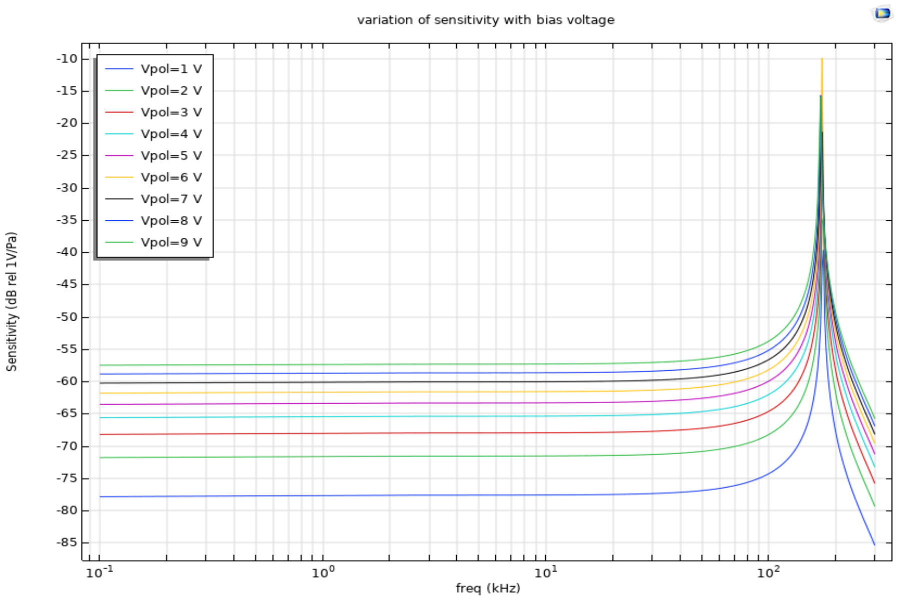
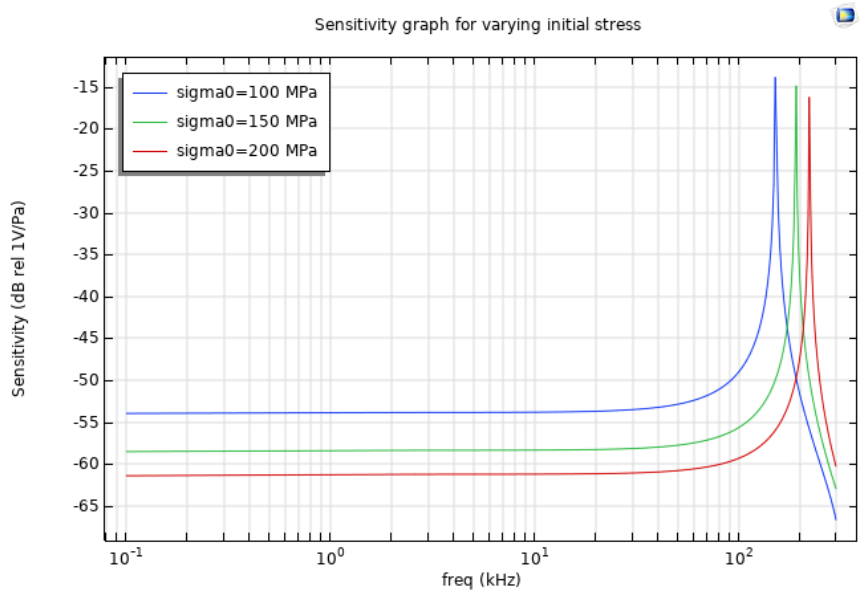


Figure 5(b): Frequency response with varying voltage

5.3. Variation of residual stress

The fabrication process of the microphone results in residual stress in the diaphragm. This cannot be controlled but it affects the performance of the microphone. As the initial stress increase, the mechanical sensitivity decreases, and therefore the open circuit sensitivity decreases as seen from the simulation. The resonant frequency is inversely proportional to the air gap and with the increase in residual stress the diaphragm displacement decreases therefore the frequency increases.



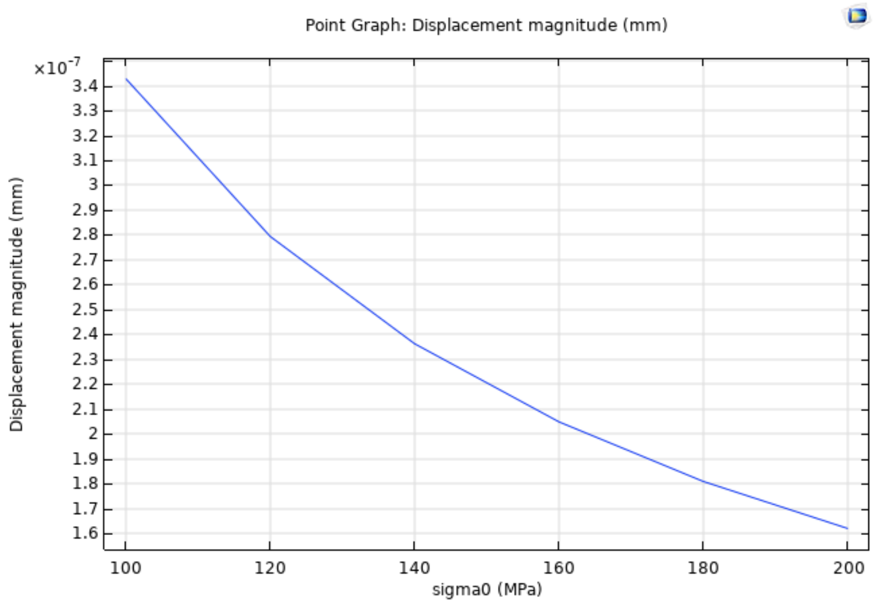


Figure 6(a) and (b): Frequency response and center displacement with varying initial stress.

5.4. Corrugated diaphragm

Geometric approach in changing or optimizing the design is an easier way to solve the initial stress issues. Corrugated membranes have been in use for a long time in the industry as they significantly reduce the initial stress in the center region of the membrane to provide improved acoustic sensitivity compared to circular clamped membranes.

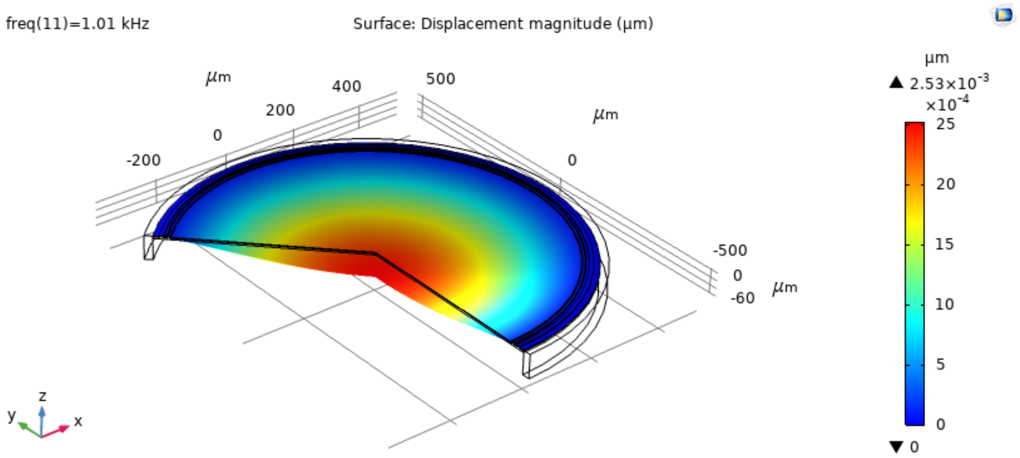


Figure 7: Displacement of corrugated circular diaphragm

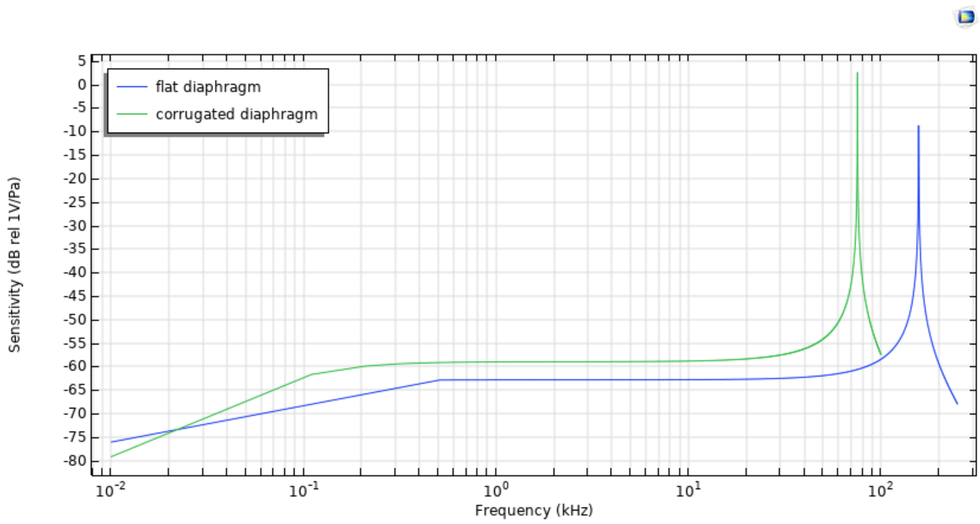


Figure 8: Frequency response of open-circuit sensitivity

The mechanical compliance for corrugated circular diaphragm can be approximately calculated by :

$$C_{corrugated} = \frac{R^2}{8t\sigma_0}\left(\frac{2Et^2}{(1-v^2)\sigma_0 R^2} + 1\right)^{-1}.\left(1 + 6sin(\beta)\frac{h_c^{\ 2}}{t^2}\frac{N_c.w_c}{R-N_c(w_c+b_c)}\right)$$

where N_c is number of corrugation, w_c is width of corrugation, b_c is distance between two corrugations, h_c is height of corrugation, and $\beta$is the angle of corrugation.
The simulation shows that the mechanical sensitivity increases with increasing corrugation height.

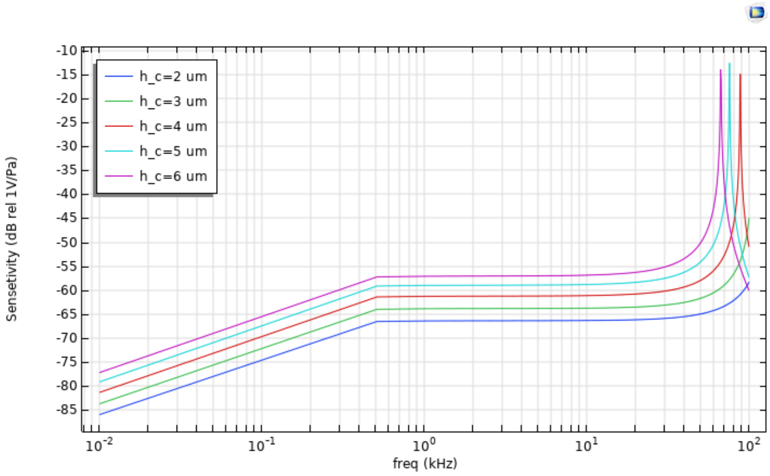


Figure 9: Frequency response with varying corrugation height

5.5 Conclusion

The simulation in COMSOL Multiphysics align with the mathematical equations. The sensitivity of the microphone can be increased by increasing bias voltage but it can be increased beyond a threshold. The other method is to increase the mechanical sensitivity which increase the overall open-circuit sensitivity of the microphone. The mechanical sensitivity increases with increase in diaphragm radius but this results in smaller bandwidth. The radius must be such that the resonance frequency lie well above the frequency of operation. In case of photoacoustic detector for trace gas sensing application, the photoacoustic signal response has frequency <20 kHz and therefore the resonant frequency should lie above 20 kHz. The microphone should also give a flat frequency response in the working range. The residual stress affects the performance of the microphone and it can't be controlled. To reduce the effect of residual stress, corrugated diaphragm is being used. The sensitivity of corrugated diaphragm microphone increases with increase in corrugation height.

6. Summary and Future Work

This report focused on the design aspect of a MEMS capacitive microphone for the application of photoacoustic detector. The report presents the theoretical principle of photoacoustic spectroscopy and the various components of the experimental setup. MEMS microphone as a detector in photoacoustic setup is studies in detail. The working of MEMS microphones and microphone specifications are explained which gives a better understanding of the design aspect of the MEMS microphones. Theoretical equation for the modeling of capacitive microphone are explained. COMSOL Multiphysics 5.6 is used to simulate the MEMS capacitive microphone and the analysis are performed to study the effect of different parameters on microphone performance. These simulations are in line with the theoretical equations and help understand the dependence of various parameters.

Future works can be done on the thermal and mechanical noise in the microphone. A detailed study on the damping in the air gap and backchamber also needs to be discussed. The thermo-viscous acoustic analysis can provide detailed information on the microphone response in the trace gas sensing application.Photoacoustic based trace gas sensing applications require high SNR but a single microphone can not improve SNR beyond a limited range. A high sensitivity requires use of low stress material to construct thin membrane with large surface area and a small air gap between the diaphragm and the back plate. The desired miniaturization is in contrast to a large membrane area. Therefore it can be advantageous to use arrays of MEMS microphone instead of one large one.

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Glossary

Acoustic - of or relating to the sense or organs of hearing, to sound, or to the science of sounds

Decibels - a relative unit of measurement equal to one-tenth of a bel.

Diaphragm - Component of the microphone capsule that vibrates in response to sound wave.

Ferroelectric - a property of certain materials to have a spontaneous polarization which can be reversed by the application of an external electric field.

Harmonic - a signal or wave whose frequency is an integral (whole number) multiple of the frequency of some reference signal or wave.

MEMS - Micro-electro-mechanical system

Microphone - a transducer that converts sound into an electrical signal.

Spectroscopy - the study of the interaction between matter and electromagnetic radiation as a function of the wavelength or frequency of the radiation.