

A COMSOL® based Illustrative Study on SAW Sensor VOC Detection for Respiratory System Issues

¹A. Nagamalli¹, Dr. D. Alli²

1. Research Scholar, Instrument Technology, ANDHRA UNIVERSITY, AUCE (A), VISAKHAPATNAM, AP, INDIA.
2. Assistant Professor, Instrument Technology, ANDHRA UNIVERSITY, AUCE(A), VISAKHAPATNAM, AP, INDIA.

INTRODUCTION Volatile Organic Compounds (VOC) which evaporate easily at room temperature. Human exhaled breath consists of more than 3000 VOCs like carbon dioxide, acetone, methanol, ethanol butane and formaldehydes. Exhaled breath analysis is a non-invasive technique adopted for the purpose of diagnosing respiratory track issues. Estimation of several gases such as acetone detection is considered, In order to achieve a SAW sensor is designed and simulated by using COMSOL Multiphysics 5.0®. Estimation Of gas sensor adsorption rate and conductivity is observed based on electric potentials, Frequency response is analyzed at various Eigen values, depends on the results obtained further characterization and fabrication of Biosensor is carried out to detect VOC thereby Human exhaled breathe Analysis can be estimated.

RESULTS: The simulated results obtained are Eigen frequency solver, from COMSOL Multiphysics 5.0® to find out the resonance frequencies. In this model, a YZ-cut LiNbO3 whose Rayleigh wave velocity (v) is around 3000 m/s. This gives an estimate of the lowest SAW frequency (f₀) to be 848 MHz and maximum Eigen value obtained is 972 MHz.

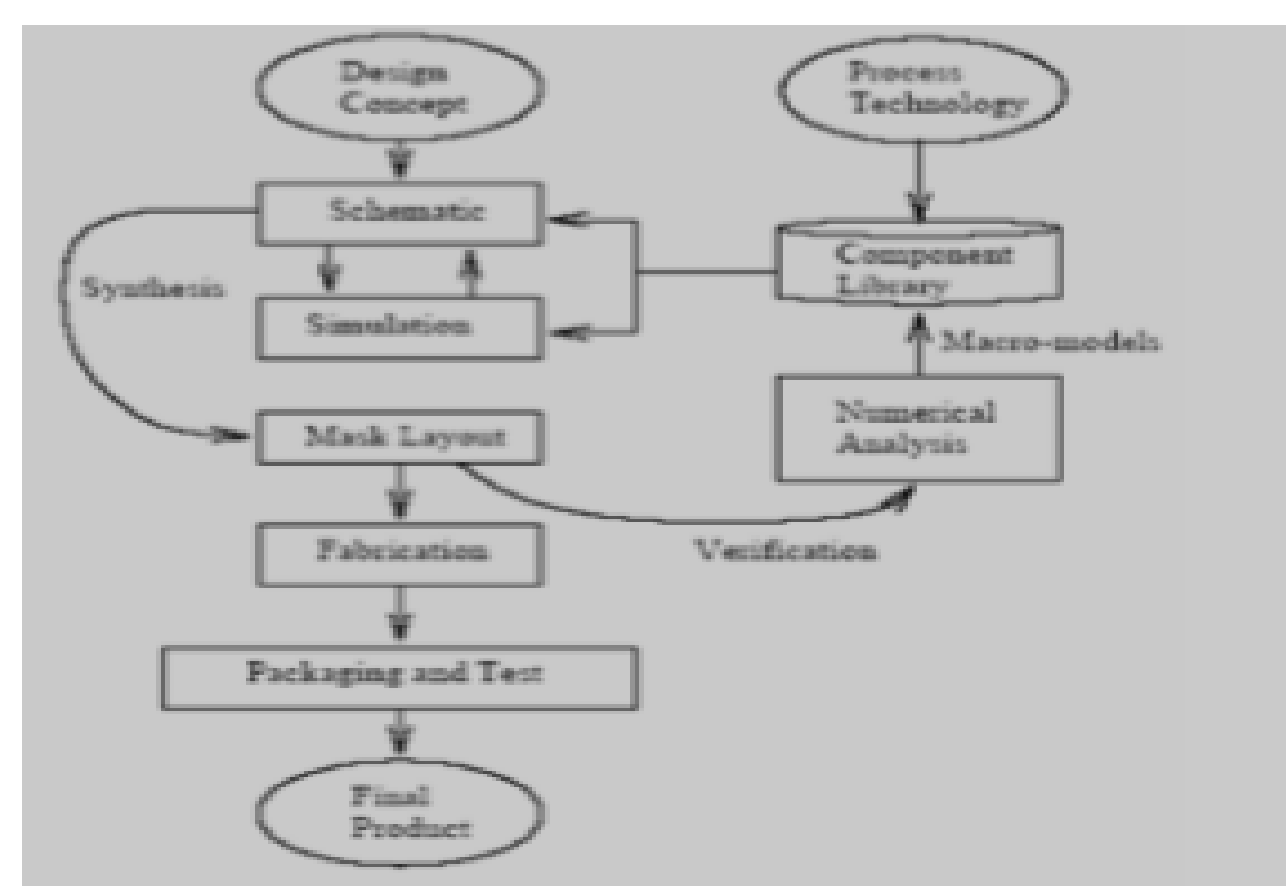


Figure 1. MEMS Design Flow

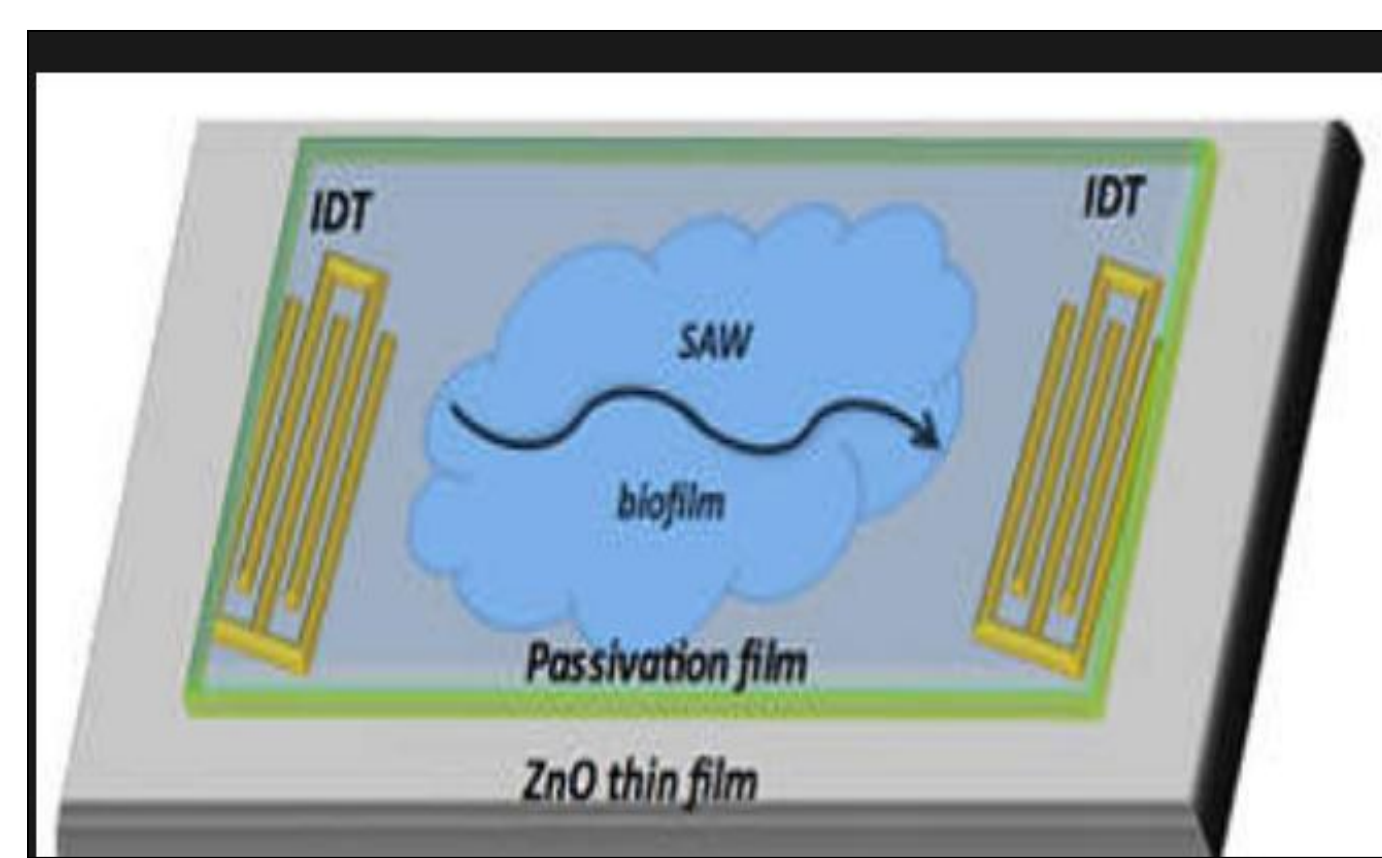


Figure 2. MEMS SAW sensor Design

COMPUTATIONAL METHODS: The simulation modeling of SAW sensor is fabricated by COMSOL Multiphysics® 5.0 The use of periodic boundary condition implies that the frequencies of interest will correspond to wavelengths that are integer fractions of the width of the geometry. The lowest SAW Eigen mode has its wavelength equal to the width of the geometry of 3 to 4 μm. Using the Rayleigh wave velocity for the given piezoelectric substrate material, estimation of resonance frequency is the main theme of this work.

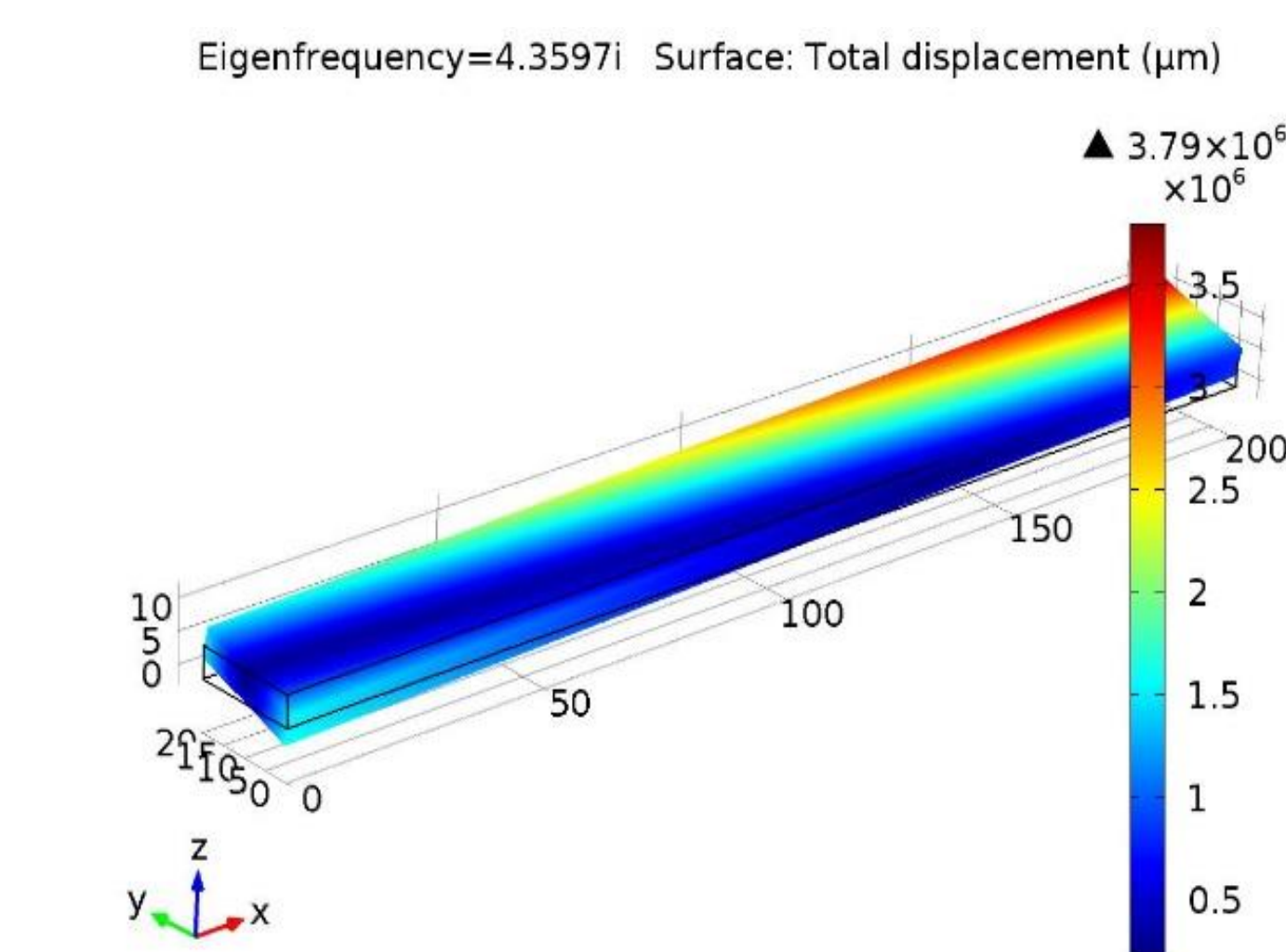


Figure 5. Simulated Rectangular Eigen frequency vs displacement

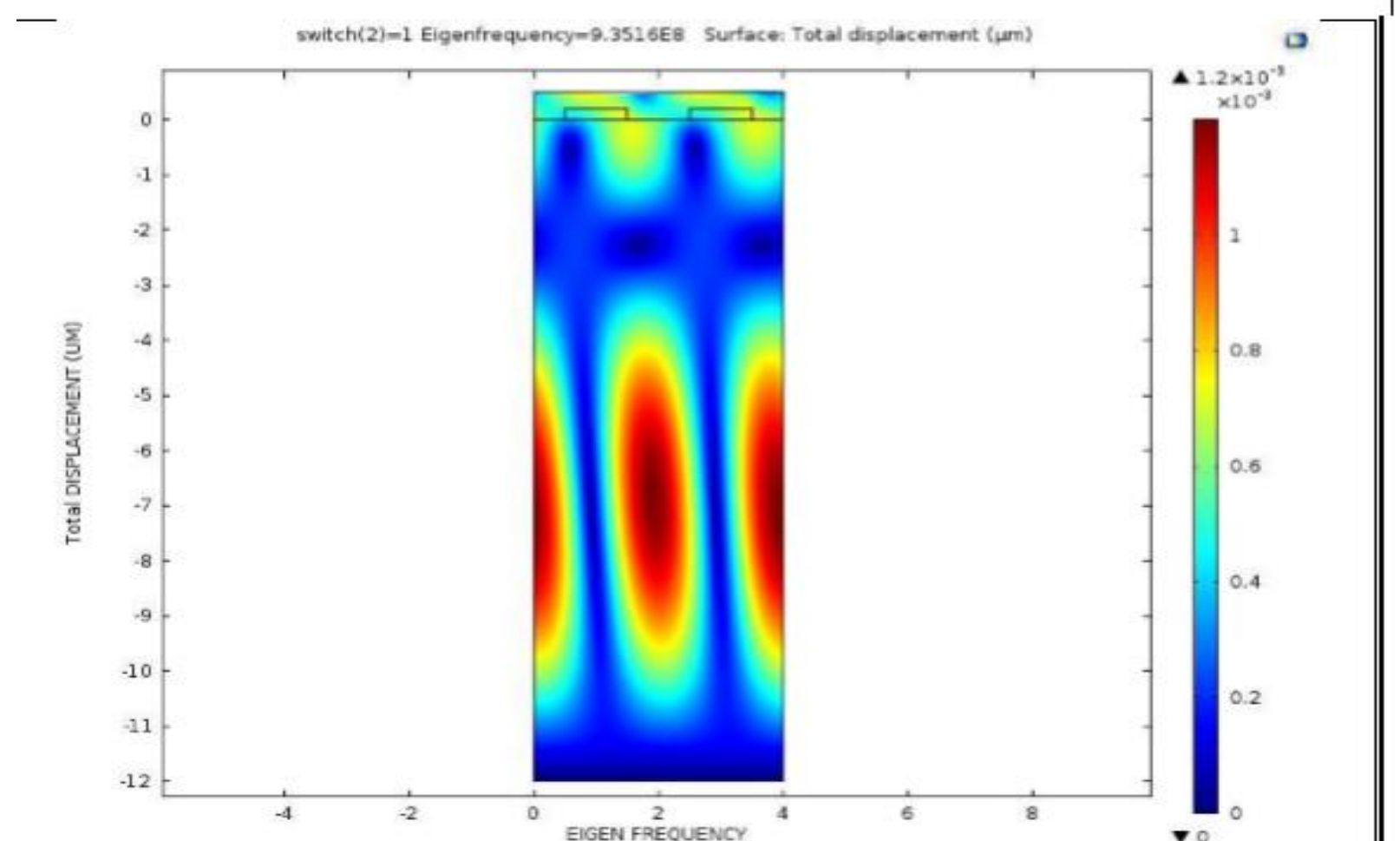


Figure 6. SAW Eigen frequency at 9.3516E8 Vs Total Surface displacement 1.28x10-3

No.	Number of boundary elements	Number of elements Resolved by meshing tetrahedral	Minimum element quality
1	154	166	0.5643
2	191	1091	0.2294
3	1196	17993	0.05709
4	1997	38018	0.01082

Table 1. FE ANALYSIS OF PZT bar

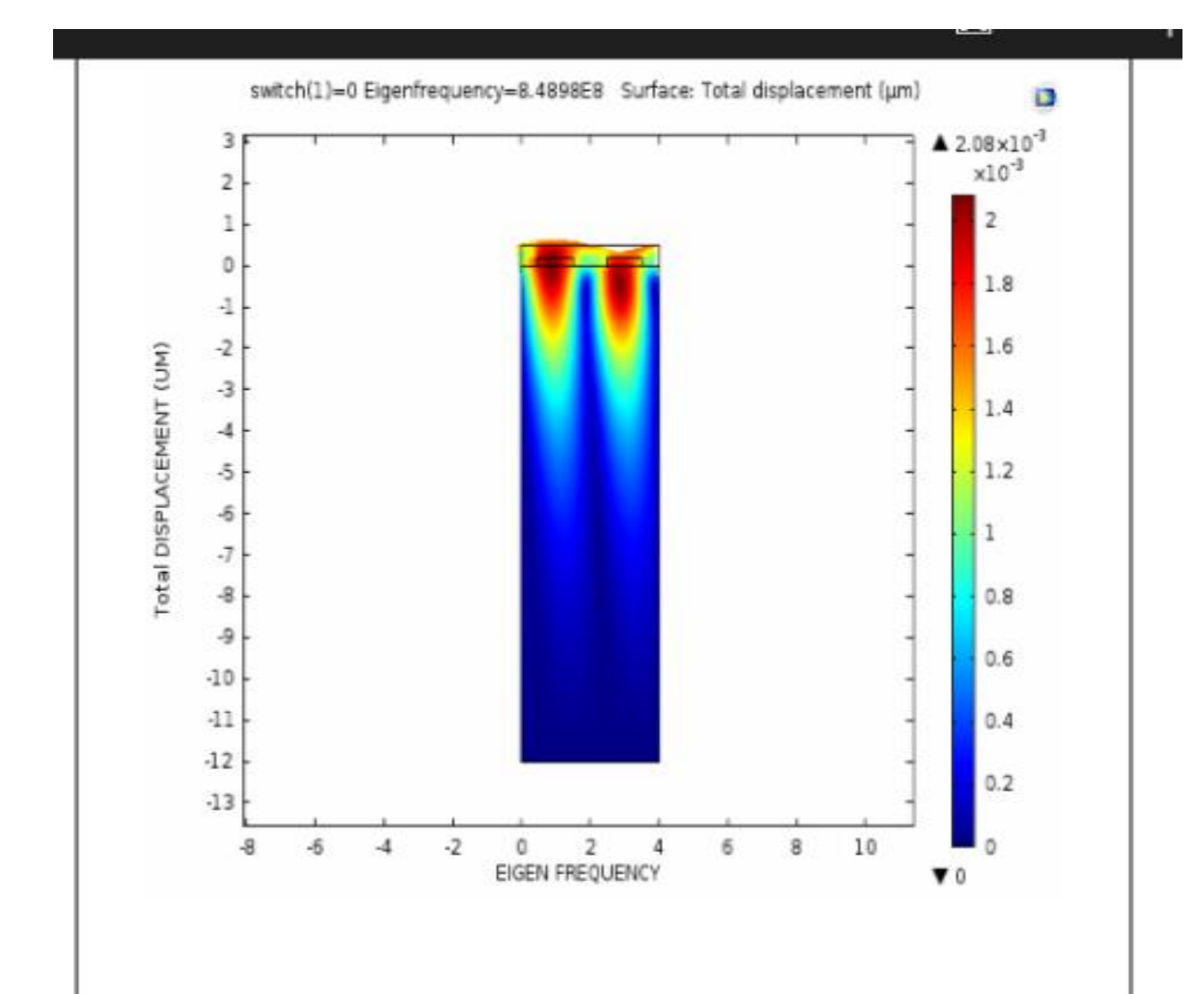


Figure 7. Switch mode (1) Eigen frequency Vs Total Displacement

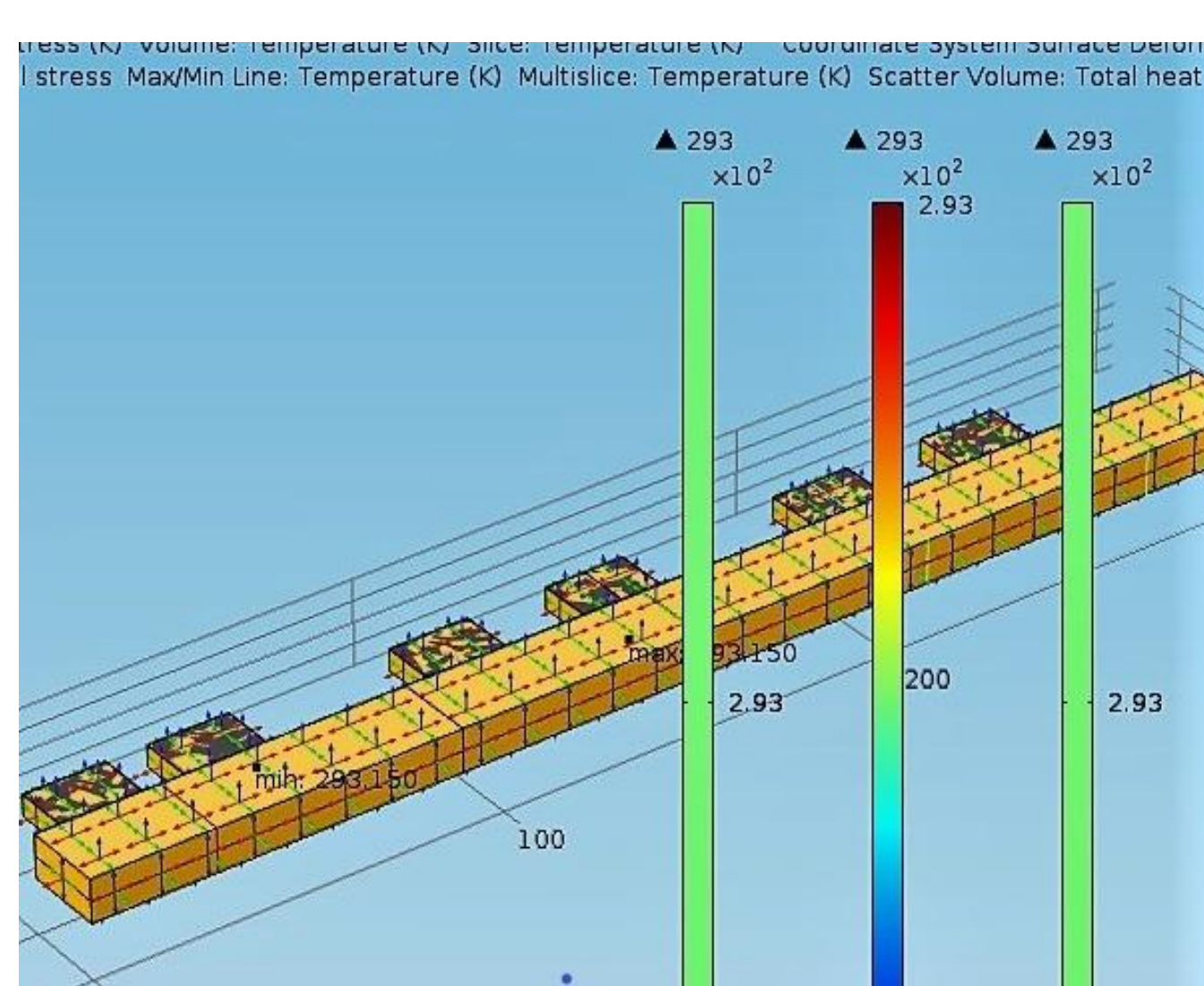


Figure 3. Comsol IDT Structure to estimate Surface roughness and Cancer Cell Progression.

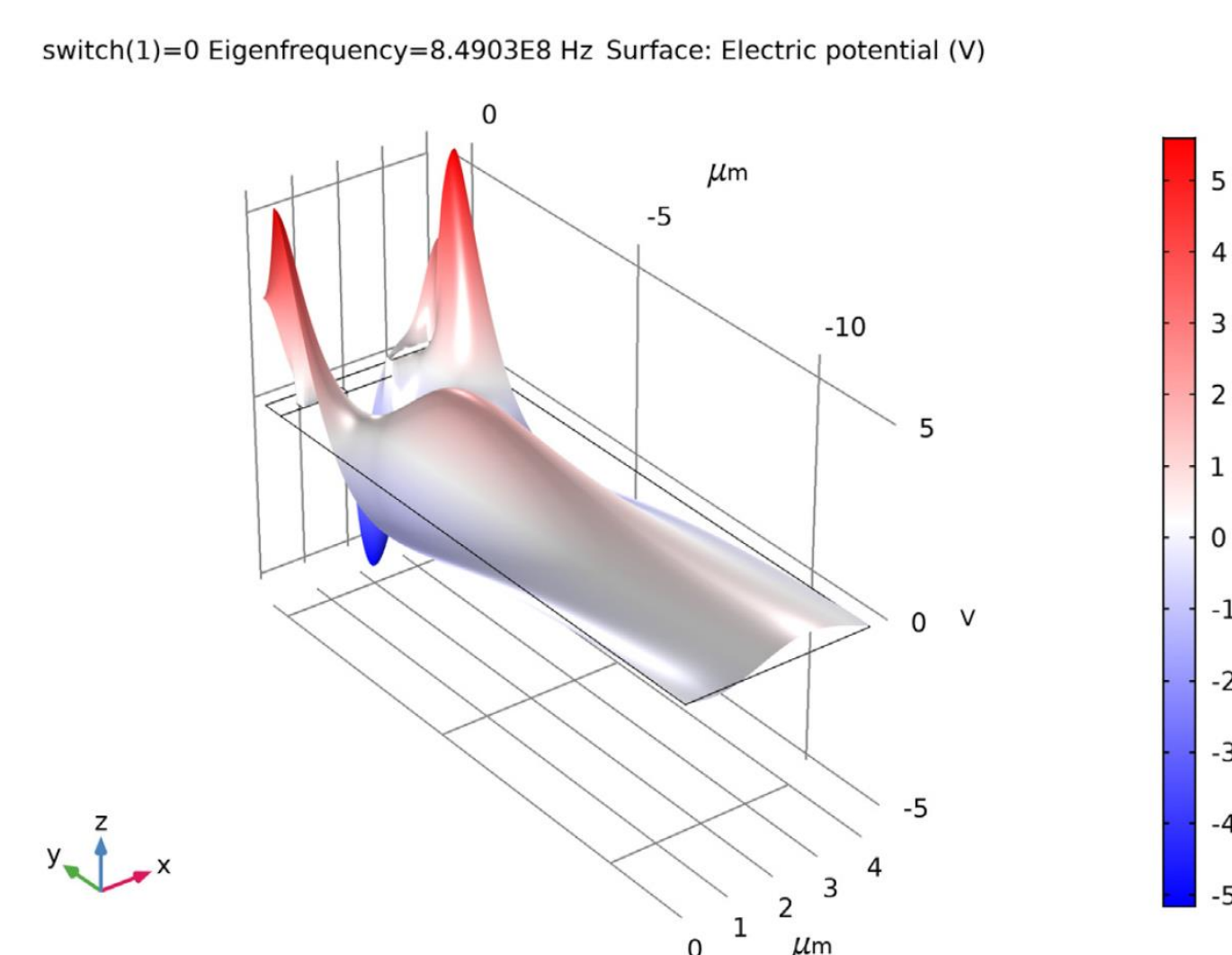


Figure 4. SAW sensor switch mode 1 Eigen frequency at 8.489E8 Vs Surface Electric potential (V)

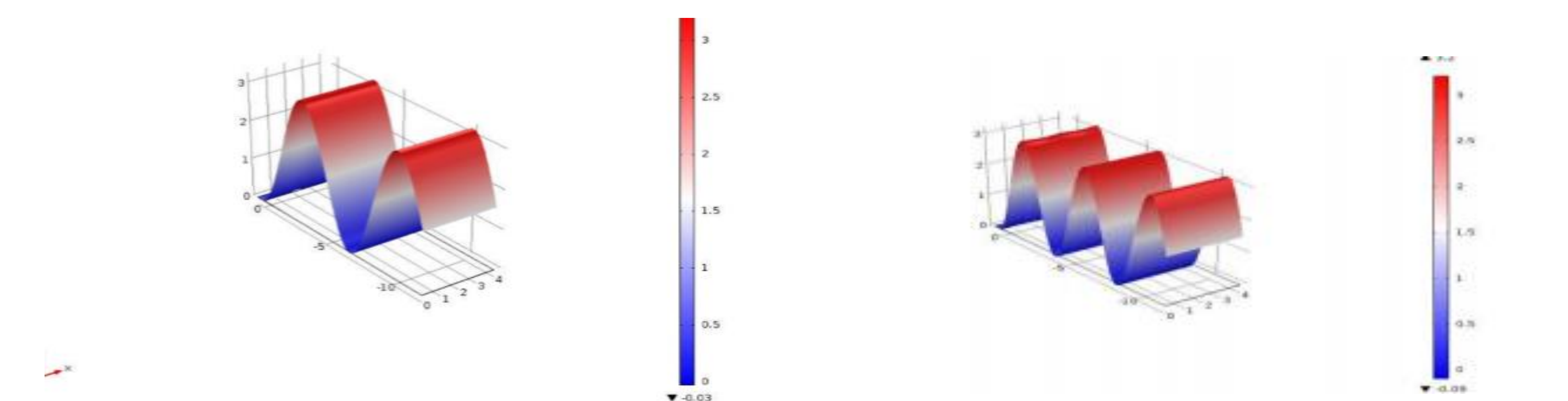


Figure 8. Switch mode (1) Eigen frequency at 9.1851E8Vs SE potential (v)
Figure 9. switch mode 1 Eigen frequency at 9.7219E8Vs SE potential (v)

CONCLUSION: MEMS VOC sensor structures designed using COMSOL Multiphysics® structural and frequency analysis applied to achieve high sensitivity, selectivity and repeatability of bio sensor. Estimation of gas sensor adsorption rate and conductivity is observed based on surface electric potentials, Frequency response is analyzed at various Eigen values, thereby detected VOCs Human exhaled breathe Analysis can be estimated and further lead to fabrication.

REFERENCES:

- [1] Jill D. Fenske & Suzanne E. Paulson "Human Breath Emissions of VOCs", Journal of the Air & Waste Management Association, 49:5, 594-598, DOI: 10.1080/10473289.1999.10463831
- [2] D. Arul, Pon Daniel ,K. Than gavel "Empirical study on Early Detection of Lung Cancer using Breath Analysis" IEEE Sponsored 2 nd International Conference on Innovations in Information, and Communication systems (ICIIECS) 2015, DOI:10.1109/ICIIECS.2015.7192869
- [3] <http://cdc.gov/nchs>, National center for disease control and prevention, 2017.
- [4] Gurusamy JT, Putrino G, Jeffery R et al., Faraone L, MEMS based hydrogen sensing with parts-per-billion resolution, *Sensors and amp; Actuators: B. Chemical*(2018).<https://doi.org/10.1016/j.snb.2018.07.118>.
- [5] Hong-Lae Kim, Jangseop Han, SM Lee et al., "MEMS-based particle detection system for measuring airborne ultrafine particles" School of Mechanical Engineering, Yonsei University, Yonsei-ro, Seodaemun-gu, Seoul, 03722, Republic of Korea© 2018 Elsevier 2018.
- [6] H. K. Gatty,G.Stemme and N. Roxhed "An ampero metric H2ssensor applicable for bad breath monitoring", Manuscript, 2015.
- [7] G. Eranna, B. Joshi, D. Runthala, and R. Gupta, "Oxide materials for development of integrated gas sensors—a comprehensive review," *Critical Reviews in Solid State and Materials Sciences*, vol. 29, pp. 111-188, 2004.
- [8] Mitsakakis, K.; Tseripi, A.; Gizeli, E. SAW device integrated with microfluidics for array-type biosensing. *Microelectron. Eng.* 2009, 86, 1416–1418.

Anisotropic piezoelectric material such as Lithium Niobate Y-Z cut, used as the Material designed with IDT structures as shown fig (2) and figure 5.

The sensitivity, S, of a gas sensing device is given by $S = dR/dn$ where R is the device response & n is the gas Concentration. The response R for an uncoated substrate is as in below equation R. Δv is change of the SAW wave velocity after gas absorption and Δm/As is the mass loading per sensitive surface unit.

$$R = \frac{\Delta v}{v} = \frac{\Delta f}{f_0} = (k_1 + k_2) f_0^2 \frac{\Delta m}{A_s}$$