DESIGN AND SIMULATION OF 3D ZnO NANOWIRE BASED GAS SENSOR FOR CONDUCTIVITY STUDIES

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Gas Sensors

- **Sensors**: Any device that senses a physical signal.
- **Gas sensor** is a subclass of chemical sensors.
- **Gas sensor**-concentration of gas.

Types of Gas Sensors

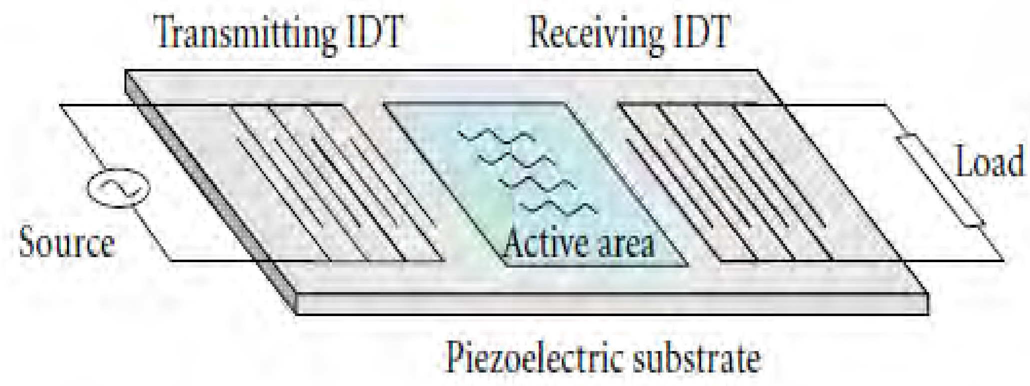
- Metal Oxide Based Gas Sensors
- Capacitance Based Gas Sensors
- Acoustic Wave Based Gas Sensors
- Calorimetric Gas Sensors
- Optical gas sensors
- Electrochemical gas sensors

Objective

- 3D gas sensor-hydrogen detection-conductivity-nanolevel
- Sensitivity increases-high surface to volume ratio
- Thickness-intermediate layer-total displacement and voltage
- Conductivity –increases and decreases.

SAW Sensor

- Two-port delay-line SAW sensor
- IDT –transmitter and receiver
- Viscoelastic properties –frequency shift and insertion loss



- Nanostructures – Active Area

Need For Nanostructure Implementation

- Acoustic energy – Minimum and Maximum
- Waveguide – Dielectric Material.
- Frequency and Wavelength

$$\lambda = 2(W_{el} + W_{sp})$$

where

W_{el} - width of each individual electrode

W_{sp} - spacing between two adjacent individual electrodes

Advantages

- Sensitivity
- Operates in high frequency (MHz to GHz)
- Elastic solid
- Surface morphology

Analytical Methods

- Types
  - Delta function model,
  - Equivalent network model,
  - Green's function model and
  - Coupling-of-mode method
- Second-order effects
  - Backscattering,
  - Diffraction
  - Mechanical loading
- Finite Element Analysis

Material Selection

Piezoelectric Substrate

- Electromechanical coefficient (K^2)
- $K^2 = 2(V_f - V_m)/V_f$

  where

  V_f - free surface phase velocity

  V_m - metallised surface phase velocity
- Polarization
- Orientation
- Lithium Niobate($LiNbO_3$)

IDTs Material

- Aluminium
- Easy to deposit
- Adheres well with the common oxide substrate

Intermediate Layer Material

- Dielectric materials –ZnO
- Lower acoustic velocity (approximately 2531 m/s)
- Properties that can influence the propagation
  - Electromechanical coupling coefficient, phase velocity, polarisation and permittivity

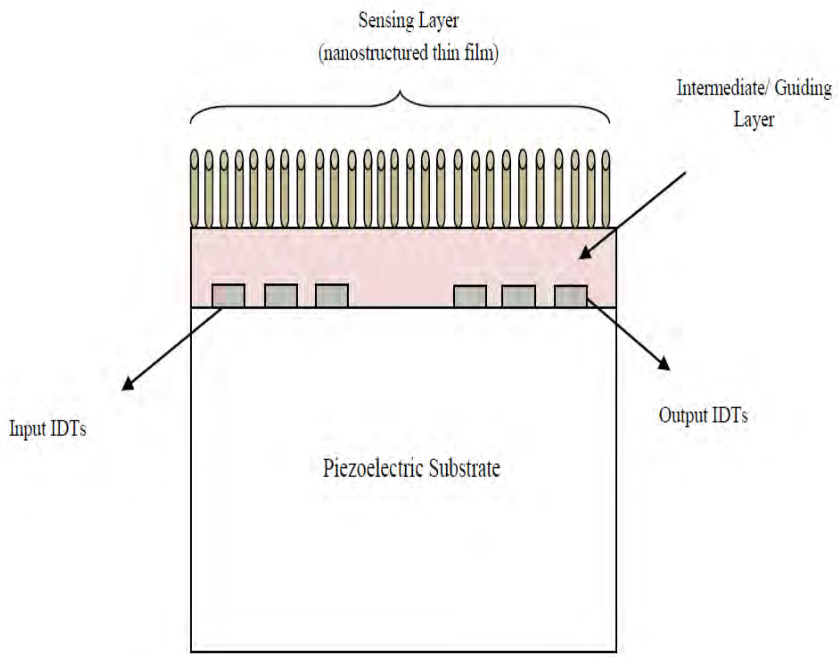
Sensing Layer Material

- Adsorption – Occurred-ZnO
- High mobility of conduction electrons
- Good thermal stability
- Chemical stability
- Good Conductivity
- Changes – Due to Adsorption

2D Gas Sensor Model

Existing Model

- Substrate –$LiNbO_3$
- IDTs- Aluminum
- Intermediate layer- ZnO
- Sensing layer –ZnO nanowire
- Optimized thickness- 1µm



Multiphysics Modeling and Structural Simulation

Modeling Dimensions

- 3D ZnO Nanowire – Hydrogen Detection
- Substrate Dimensions
  - 30µm in the *X*-axis
  - 10µm in the *Y*-axis and
  - 4µm in the *Z*-axis.
- Intermediate layer Dimensions
  - 30µm in the *X*-axis
  - 10µm in *Y*-axis and
  - 1µm in the *Z*-axis

Contd..

- IDTs Dimensions
  - 1μm as the width
  - 0.2μm as the height

- Sensing Layer Dimensions
  - ZnO nanowires 0.1μm as the radius
  - 2.5μm as the height

Geometry

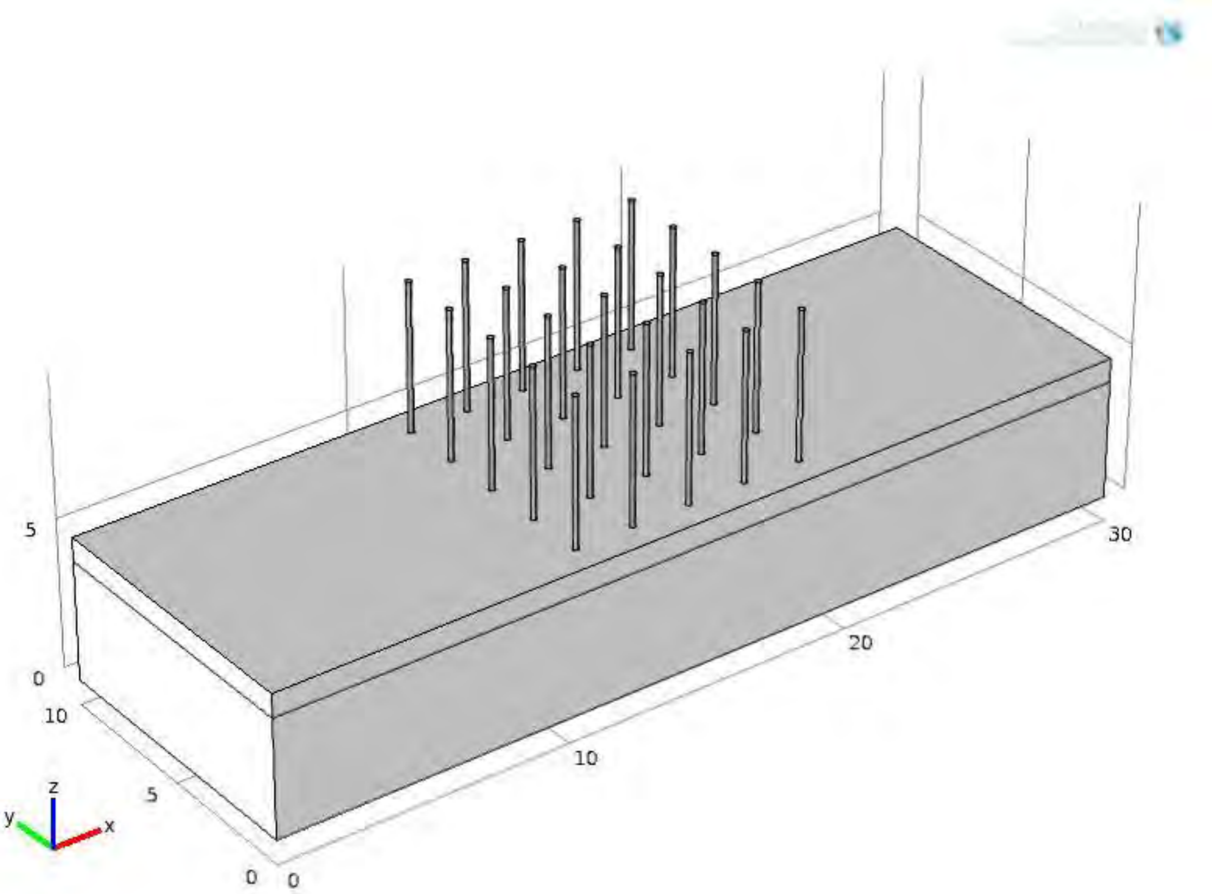


Fig: SAW Sensor with Nanowire as the Sensing Material

Structural Simulation

- Analysis – Piezoelectric Studies
  - Boundary 3 – Fixed Constraint
  - First and Third electrode – Electrical Potential
  - Second and Fourth electrode – Zero Potential

$$rho\_ZnO + rho\_H2\_ZnO = 5676\ kg/m^3 + 1.647871 \times 10^{-6}\ kg/m^3$$

- Meshing – Free tetrahedral

Mesh Model

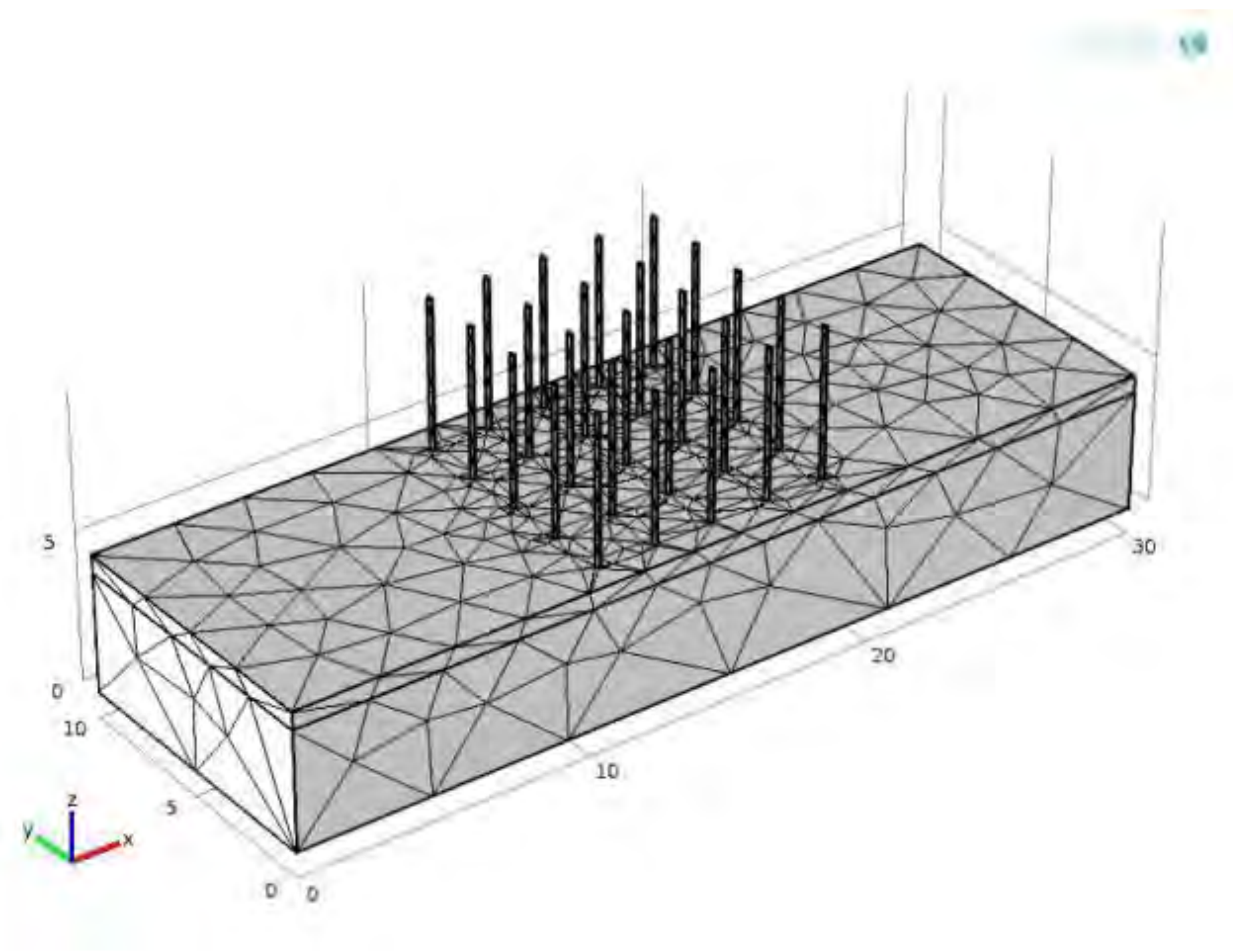


Fig: Completed Mesh Model

Results and Discussion

- Focussed - total displacement and voltage contour.
- Different Thickness of Intermediate layer
    - 0.4μm, 0.6μm, 0.8μm, 1.0μm, 1.2μm, 1.6μm, 1.8μm and 2.0μm

Simulation Result

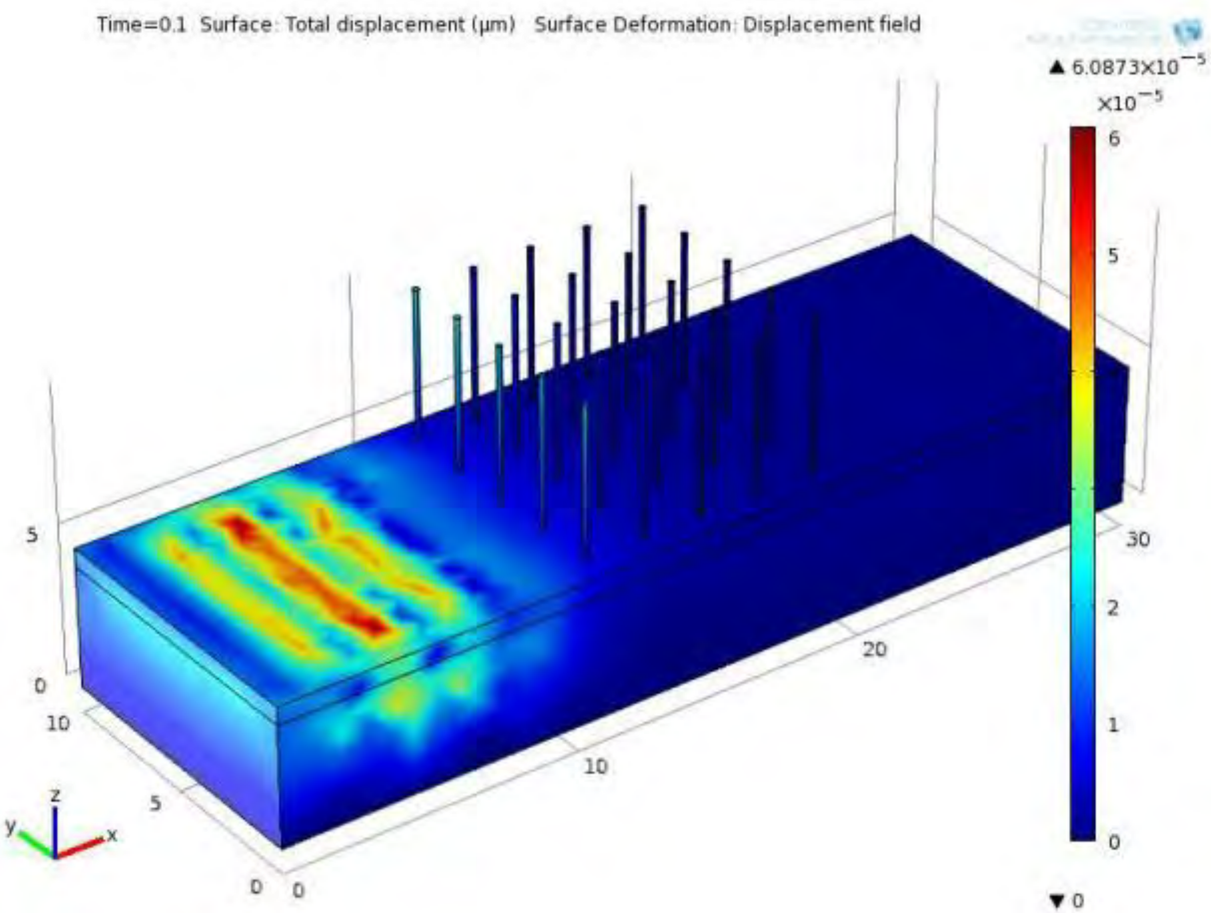


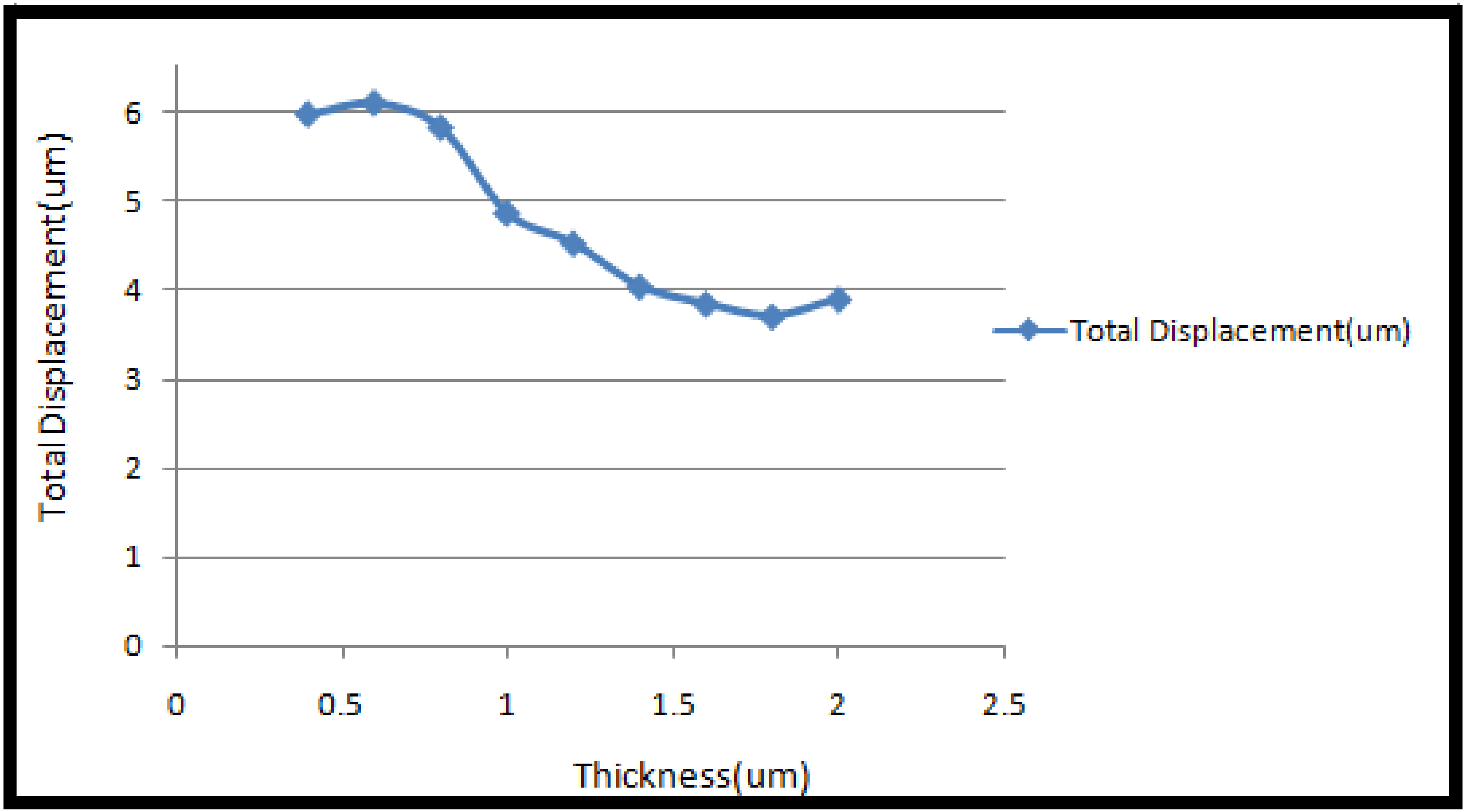
Fig: Simulation result of 0.6μm Thickness of ZnO layer

Tabulation

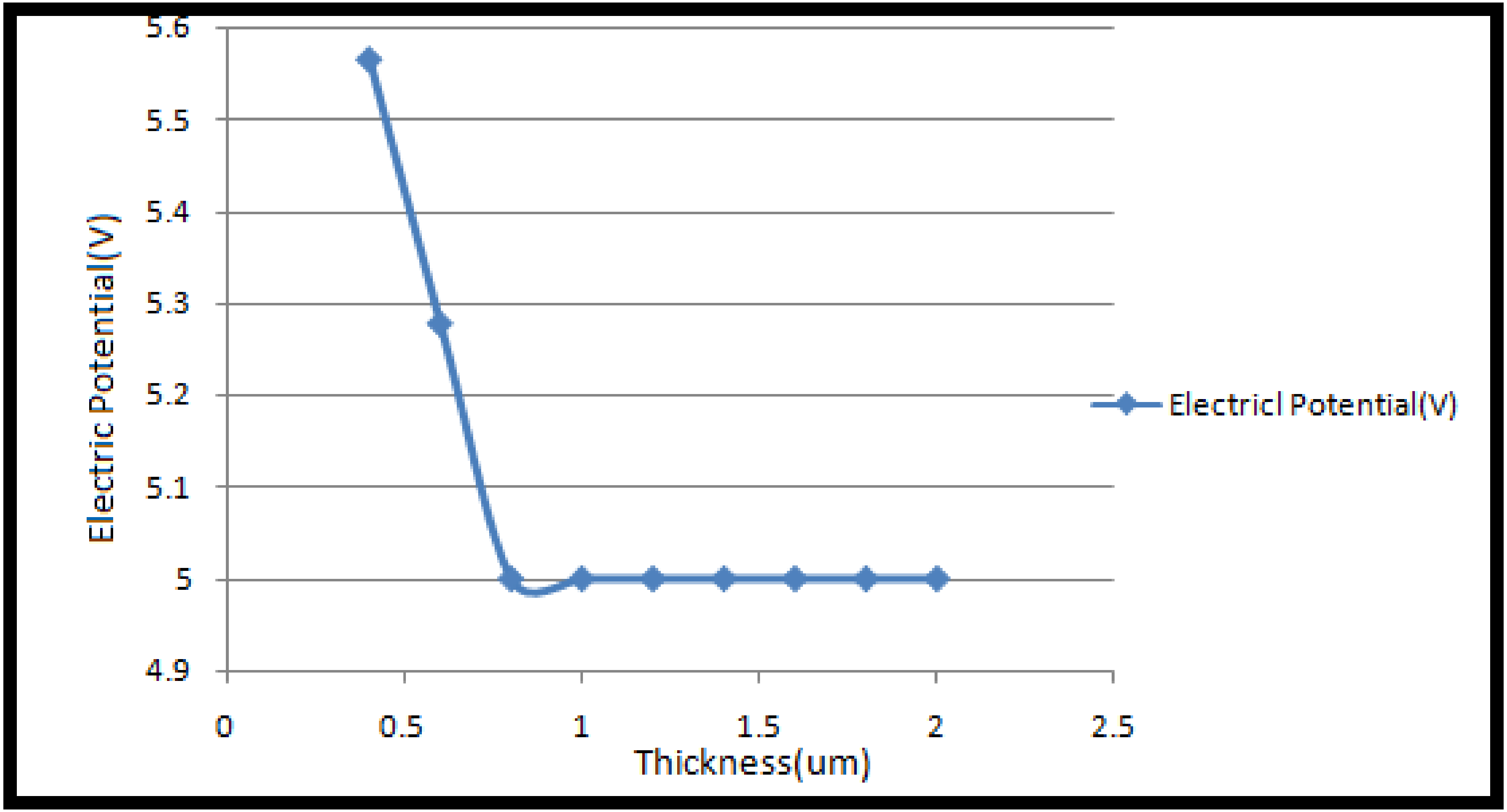
Intermediate Layer Thickness(μm)	Total Displacement(10^{-5}m)	Electric Potential(V)
0.4	$5.9625*10^{-5}$	5.565
0.6	$6.0873*10^{-5}$	5.2777
0.8	$5.8539*10^{-5}$	5
1.0	$4.8625*10^{-5}$	5
1.2	$4.5234*10^{-5}$	5
1.4	$4.0416*10^{-5}$	5
1.6	$3.8492*10^{-5}$	5
1.8	$3.7092*10^{-5}$	5
2.0	$3.9007*10^{-5}$	5

Total Displacement and Electric Potential for different Thickness of Intermediate Layer

Plot of Different Thickness of ZnO layer vs Total Displacement Obtained



Simulation Result of Voltage Contour via different thickness



Applications

- Coolant in generators
- Fuel of future
- Aerospace industry
- Batteries and Fuel cells
- Chemical industries

Conclusion

- Modeled 3D Gas Sensor
- Optimised Thickness – 0.6μm
- Enhanced Performance

References

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