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 – LiNbO₃
- 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
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
Fig: SAW Sensor with Nanowire as the Sensing Material
Analysis – Piezoelectric Studies

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

\[ \text{rho}_\text{ZnO} + \text{rho}_\text{H2}_\text{ZnO} = 5676 \text{ kg/m}^3 + 1.647871 \times 10^{-6} \text{ kg/m}^3 \]

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

<table>
<thead>
<tr>
<th>Intermediate Layer Thickness(μm)</th>
<th>Total Displacement($10^{-5}$m)</th>
<th>Electric Potential(V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>$5.9625\times10^{-5}$</td>
<td>5.565</td>
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<tr>
<td>0.6</td>
<td>$6.0873\times10^{-5}$</td>
<td>5.2777</td>
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<td>0.8</td>
<td>$5.8539\times10^{-5}$</td>
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<td>1.0</td>
<td>$4.8625\times10^{-5}$</td>
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<td>1.2</td>
<td>$4.5234\times10^{-5}$</td>
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</tr>
<tr>
<td>1.4</td>
<td>$4.0416\times10^{-5}$</td>
<td>5</td>
</tr>
<tr>
<td>1.6</td>
<td>$3.8492\times10^{-5}$</td>
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</tr>
<tr>
<td>1.8</td>
<td>$3.7092\times10^{-5}$</td>
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</tr>
<tr>
<td>2.0</td>
<td>$3.9007\times10^{-5}$</td>
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</tr>
</tbody>
</table>

Total Displacement and Electric Potential for different Thickness of Intermediate Layer

11/17/2011
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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