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

Gouthami.N[*,1], Parthiban.D[1],Alagappan. M[1] and Anju.G[1]
[1] PSG College of Technology, Coimbatore, Tamil Nadu, India
*gouthami.20@gmail.com

Abstract: The objective of this paper is to design a 3D Gas Sensor for sensing Hydrogen gas and to increase the conductivity at nano level. In this novel design, nanowire acts as the sensing layer. The sensitivity towards gas adsorption is found to be increased due to its high surface to volume ratio. By varying the thickness of the intermediate layer (ZnO), there is an increase in the total displacement and voltage, higher sensitivity and mechanical robustness because it prevents energy loss into the bulk of substrate. The conductivity is found to be increasing till a certain value of the intermediate thickness after which it starts decreasing. Hence the intermediate layer thickness has to be optimized to obtain suitable conductivity. Also the use of ZnO nanowires on the sensing layer enhances the conductivity. Thus this sensor acts as a better device for sensing the amount of hydrogen gas in the atmosphere.

Keywords: SAW, ZnO NanoStructures, IDTs, 3D modeling, Hydrogen Gas.

1. Introduction

Surface Acoustic Wave (SAW) is the confinement of acoustic energy in which the energy is more sensitive near the surface of device. SAW device is widely used due to its small size, inherently rugged, inexpensive, and sensitivity in which they respond to most gases[1].

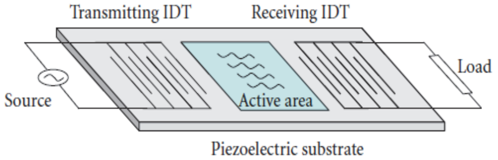

Fig.1. Model of Surface Acoustic Wave Sensor

To use this device as a gas sensor, a two port delay-line configuration is used. In such a two-port delay-line SAW sensor, two sets of interdigitated transducers (IDTs) placed a top of a piezoelectric substrate are necessary for generating and receiving acoustic waves. The first set of IDTs is called the transmitter and the second set the receiver. The transmitter converts an alternating electrical signal into an acoustic wave which travels along the surface of the piezoelectric substrate, and the receiver converts the acoustic wave back to an electrical signal for detection and analysis. The area between the generator and receiver is often coated with a chemically sensitive surface for molecular absorption or adsorption. SAW sensors can be used to detect molecular absorption and adsorption events or changes in the viscoelastic properties of the sensitive surface by measuring the wave characteristics such as frequency shift and insertion loss. In view of this, we incorporated nanostructures to increase the active area of the sensor to enhance the detection performance[2]. Here, wave properties like acoustic wave total displacement and voltage contour towards gases will be focussed.

1.1 Need for Nanostructure Implementation

To achieve high sensitivity in gas sensors, it is essential to confine a maximum amount of acoustic energy near the surface of the substrate and minimize wave scattering into the bulk of the substrate. For this, a waveguide layer made of a dielectric material, is used to confine acoustic energy close to the surface of the device. Dielectric materials act as good waveguide materials. The frequency of operation is governed by $f_o = v_o/\lambda$, where λ is the wavelength of the acoustic wave which is given by $\lambda = 2(W_{el} + W_{sp})$, where W_{el} ,W_{sp} represent width of each individual electrode and spacing between two adjacent individual electrodes, v_o is the travel velocity of the acoustic wave in the piezoelectric material. The nanostructures added to the active surface of SAW sensors can be categorized namely dispersed nanoparticles and nanoparticle conjugates, random nanofibers, nanobelts, nanotubes, standing nanostructures and porous nanostructures.

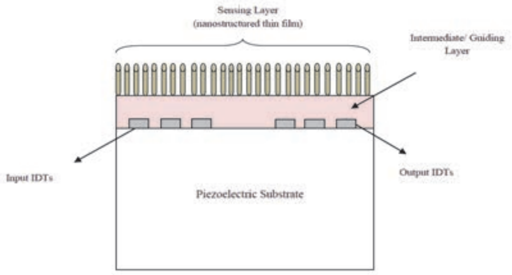

Fig.2. 2D Nanostucture Enhanced Gas Sensor

Apart from trapping the acoustic energy close to surface, it is essential to increase the area of the active surface for higher molecular absorption. For this, nanostructures are added to the active area of the sensor due to their higher surface to volume ratio. Here, the sensitivity can be optimised by varying the thickness of intermediate layer. On the other hand, it can also operate in high frequency ranges (MHz to GHz), thus becoming highly sensitive to surface perturbation and changes of an elastic solid. Adding nanostructures to the active surface of a SAW sensor will change the surface morphology, which in turn would add scattering loss and affect profoundly the behavior of wave propagation. To elucidate this impact it is imperative that the effect of adding standing nanostructures on the wave propagation and detection sensitivity be investigated analytically.
Various analytical methods have been used to study the underlying mechanism for SAW propagation. Among these methods, the delta function model, equivalent network model, Green’s function model and coupling-of-mode method are most notable. For instance, the Green’s function method was applied to determine material parameters such as elastic constants and density in nanostructures[1]. Generally, these methods are able to address certain design issues associated with SAW devices, but they cannot predict the full-scale behavior of these SAW devices. In these models, the second-order effects such as backscattering, diffraction and mechanical loading have either been ignored or simplified, thus making it highly difficult to predict the behavior of the SAW devices for high-frequency applications where the second-order effects are significant.

1.2 Material Selection

1.2.1 Piezoelectric Substrate Material

The substrate chosen are determined by some specification such as electromechanical coefficient (K^2), polarization and orientation. The propagation of the wave, interacts with the energy conversion between the electrical energy and mechanical energy that will result in efficiency measurement or (K^2) which is determined by $K^2 = 2(V_f - V_m)/V_f$ where V_f and V_m represents free surface and metallised surface phase velocities[1]. The most common substrate material always used are Lithium Niobate ($LiNbO_3$) and Lithium Tantalate ($LiTaO_3$) because have relatively high K^2. However need to consider the mode of SAW before choosing because it has different acoustic properties in which each of them will provide the differences criteria with conductivity based sensitivity.

1.2.2 IDTs Material

Aluminium has been chosen as IDTs material because it is easy to deposit and adheres well with the common oxide substrate compared to other material like gold (Au) and chromium (Cr).

1.2.3 Intermediate Layer Material

Dielectric materials such as silicon dioxide, Zinc Oxide, parylene, polymethylmethacrylate, photoresists, novolac resin are good waveguide materials. The material chosen for the intermediate layer is ZnO which will interact with piezoelectric substrate material. The reason of choosing ZnO is because it has lower acoustic velocity (approximately 2531 m/s) compared to other dielectric intermediate materials. The addition of ZnO layered on top of $LiNbO_3$ will give impact towards the acoustic wave properties. Some properties that can influence the propagation are electromechanical coupling coefficient, phase velocity, polarisation and permittivity. Here, the ZnO intermediate layer needs to be varied in thicknesses so that it can react towards gas adsorption that will affect K^2 as well[1-2].

1.2.4 Sensing Layer Material

Sensing mechanism is very important during the perturbation to make sure that adsorption has occurred. Hence, ZnO has been chosen as sensing layer also to interact with the gas analyte. The factor of high mobility of conduction electrons and have combination of good thermal and chemical stability. Here, ZnO nanowire is very much useful in sensor applications mainly due to its unique electronics properties. It has a very good conductivity when compared to other nanostructured elements. There is a deformation due to the absorption of the gas molecules on the nanowire which results in change of conductivity. Thus, with the help of change in conductivity it can be used in sensor applications which will offers promising result.

2. Governing Equations

The propagation of acoustic waves in a piezoelectric material is governed by the following coupled electromechanical constitutive equations:

$$T= C_E \bullet S - et \bullet E, \quad (1)$$
$$d = e \bullet S + \varepsilon \bullet E, \quad (2)$$

where T is the stress tensor, C_E is the stiffness matrix, S is the strain tensor, e is the piezoelectric coupling tensor, E is the electric field vector, d is the electrical displacement, ε is the dielectric matrix, and the superscript t represents the transpose of a matrix[1,4]. These constitutive equations can be related to the applied electrical potential and the induced mechanical displacements by applying Newton's law for mechanical movements and Gauss's law for electrostatic movements. According to Newton's second law of motion, the stress can be expressed as $\nabla \bullet T = \rho \ddot{u} - F$, where ρ is the density of the substrate material, $\ddot{u}$ is the particle acceleration, and F is the mechanical force. Since there is no internal or external force acting on the substrate, this equation reduces to $\nabla \bullet T=\rho \ddot{u}$. Based on Gauss's law, the electrical displacement can be expressed as $\nabla \bullet d = 0$ when the electrical charge density is zero. Moreover, in a linear material, the electrical displacement is directly proportional to the electric field $d = \varepsilon E$. This equation can be further written as $d = -\varepsilon \nabla \phi$ after applying $E = -\nabla \phi$, where ϕ is the electric potential. Moreover, the linear strain displacement relationship can be written as $S = (\nabla u + \nabla \ddot{u})/2 = \nabla su$. With these relationships, the constitutive equation (1) can be expressed in terms of the applied potential (ϕ) and the induced mechanical displacement and acceleration (u and $\ddot{u}$) along with the material properties (CE, et, and ε) as

$$\nabla \bullet [e^t \bullet \nabla \varphi] + \nabla \bullet [C_E \bullet \nabla_s u] - \rho \ddot{u} = 0$$

$$\nabla \bullet [e^t \bullet \nabla_s u] = \nabla \bullet [\varepsilon \bullet (\nabla \varphi)]$$

3. Multiphysics Modeling

Fig.3 shows a 3D representation of the SAW ZincOxide Nanowire based gas sensor for sensing hydrogen. The dimensions of the piezoelectric substrate are 30μm in the *X*-axis, representing the width of the substrate, 10μm in the propagating *Y*-axis and about 4μm in the *Z*-axis. The dimensions were chosen due to the limitations on the number of nodes which the software can generate. Intermediate layer of ZnO with size of 30μm in the *X*-axis, representing the width,10μm in *Y*-axis and about 1μm in the *Z*-axis is placed above the piezoelectric substrate. Standing ZnO nanowires with the size of 0.1μm as the radius and 2.5μm as the height are placed at the center in between the input and output ports. The dimensions of the IDTs are 1μm as the width and 0.2μm as the height. The IDTs were defined on the piezoelectric substrate as massless electrodes so that the second order effects of the electrodes can be ignored to simplify the computation.

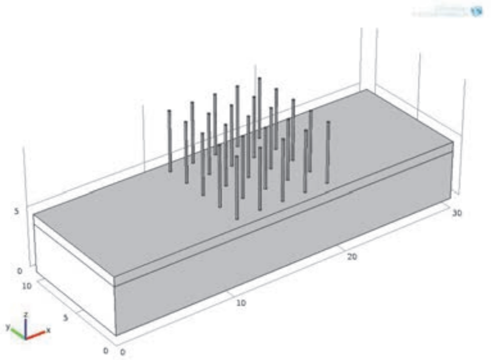

Fig.3. SAW Sensor with Nanowire as the Sensing Material

4. Structural Simulation

Here the analysis is done by considering 3D Piezoelectric Studies of FEM COMSOL Multiphysics 4.1. The boundary settings will set the boundary condition (BC) of mechanical BC and electrical BC of interface between the model geometry and its surrounding which include interior and exterior boundaries. All exterior boundaries of the mechanical BC are set to free, except boundary 3 that is set to be fixed. Meanwhile for the electrical BC, all exterior condition is set as zero charge. For input IDTs, first and third electrodes are set to electrical potential of 5V, meanwhile second and fourth electrodes are kept as default zero potential. The output IDTs are set to zero charge but the bottom of electrodes are set to be zero potential. For simulation Free Tetrahedral Meshing process and Size as Extra Coarse is chosen to determine the nodes in the structure whereby the highest density of nodes was directly under IDTs location and at the centre of the structure as in Figure.4.

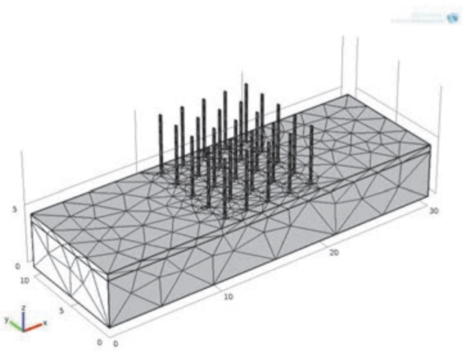

Fig.4. Mesh Model

5. Results and Discussion

The analysis is explained with the help of SAW properties like total diaplacement and voltage contour. Here, thickness of ZnO intermediate layer is varied to find the best thickness layer for the optimum sensitivity. The device was modeled with different ZnO intermediate thickness such as 0.4µm, 0.6µm, 0.8µm, 1.0µm, 1.2µm, 1.6µm, 1.8µm and 2.0µm respectively. The simulation was done with a time of 0.1sec. Results after being exposed to hydrogen gas with nanostructure as the sensing layer is shown in the Figure.5.

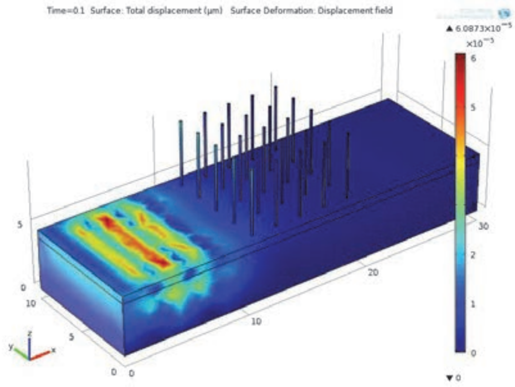

Fig.5. Simulated result of 0.6µm Thickness of ZnO layer

The graphs were plotted between Total Displacement and Thickness of the Intermediate layer (shown in Fig 6) and the voltage contour vs Thickness (shown in the Fig 7). It is clearly seen that 0.6µm has the higher total displacement values among other thickness values which shows better sensitivity. The voltage gets decreased as thickness increases and then suddenly after a particular thickness voltage becomes constant. This shows that the voltage is more concentrated on the surface.

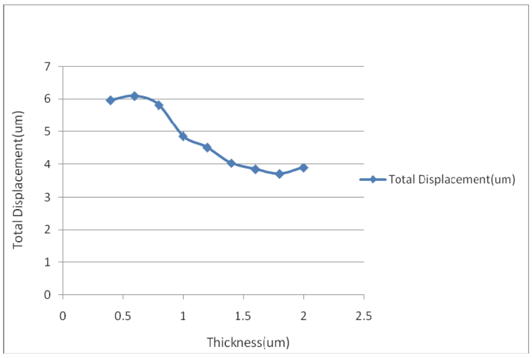

Fig.6. Plot of Different Thickness of ZnO layer vs Total Displacement Obtained.

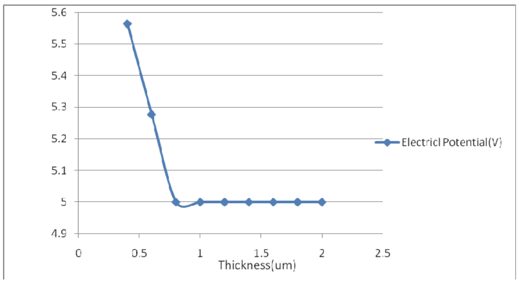

Fig.7. Simulated Result of Voltage Contour via different thickness

5. Conclusions

A 3D Multiphysics Modeling of ZnO nanowire based gas sensor was done to investigate its performance for Hydrogen Sensing and increased conductivity. As a result, this device shows higher sensitivity and prevents energy loss into the bulk of substrate. Hence, different thicknesses of ZnO intermediate layer show different sensing performance after being exposed to H_2 gas. The optimised thickness was found to be 0.6µm.The same model when simulated in 2D, concluded 1µm as the optimised thickness. Hence, ZnO nanowires are seen to enhance the performance of sensor due to high surface to volume ratio and reduce the thickness to 0.6µm in the 3D simulation.

6. References

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